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| (51) International Patent Classification ⁶ : C12N 9/28, A21D 8/04 | A1 | (11) International Publication Number: WO 99/43794 (43) International Publication Date: 2 September 1999 (02.09.99) |
| (21) International Application Number: PCT/DK99/00088 (22) International Filing Date: 26 February 1999 (26.02.99) (30) Priority Data: 0269/98 27 February 1998 (27.02.98) DK 60/077,795 12 March 1998 (12.03.98) US (71) Applicant (for all designated States except US): NOVO NORDISK A/S [DK/DK]; Novo Allé, DK-2880 Bagsværd (DK). (72) Inventors; and (75) Inventors/Applicants (for US only): CHERRY, Joel, Robert [US/US]; 916 Anderson Road, Davis, CA 95616 (US). SVENDSEN, Allan [DK/DK]; Bakkeledet 28, DK-3460 Birkerød (DK). ANDERSEN, Carsten [DK/DK]; Højeloft Vænge 162, DK-3500 Værløse (DK). BEIER, Lars [DK/DK]; Skeltoftevej 16, st. h, DK-2800 Lyngby (DK). FRANDSEN, Torben, Peter [DK/DK]; Alhambravej 22, 1, th, DK-1826 Frederiksberg C (DK). (74) Common Representative: NOVO NORDISK A/S; Corporate Patents, Novo Allé, DK-2880 Bagsværd (DK). | | (81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG). Published <i>With international search report.</i> |
| (54) Title: MALTOGENIC ALPHA-AMYLASE VARIANTS (57) Abstract The inventors have modified the amino acid sequence of a maltogenic alpha-amylase to obtain variants with improved properties, based on the three-dimensional structure of the maltogenic alpha-amylase Novamyl. The variants have altered physicochemical properties, e.g. an altered pH optimum, improved thermostability, increased specific activity, an altered cleavage pattern or an increased ability to reduce retrogradation of starch or staling of bread. | | |

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MALTOGENIC ALPHA-AMYLASE VARIANTS

FIELD OF THE INVENTION

The present invention relates to variants of maltogenic amylase and to methods of constructing such variants.

5 BACKGROUND OF THE INVENTION

Maltogenic alpha-amylase (glucan 1,4- α -maltohydrolase, E.C. 3.2.1.133) is able to hydrolyze amylose and amylopectin to maltose in the alpha-configuration, and is also able to hydrolyze maltotriose as well as cyclodextrin.

A maltogenic alpha-amylase from *Bacillus* (EP 120 693) is commercially
10 available under the trade name Novamyl® (product of Novo Nordisk A/S, Denmark) and is widely used in the baking industry as an anti-staling agent due to its ability to reduce retrogradation of starch. Novamyl® shares several characteristics with cyclodextrin glucanotransferases (CGTases), including sequence homology (Henrissat B., Bairoch A. 1996) and formation of transglycosylation products (Christophersen, C., et al., 1997,
15 Starch, vol. 50, No. 1, 39-45).

Cyclomaltodextrin glucanotransferase (E.C. 2.4.1.19), also designated cyclodextrin glucanotransferase or cyclodextrin glycosyltransferase, abbreviated herein as CGTase, catalyses the conversion of starch and similar substrates into cyclomaltodextrins via an intramolecular transglycosylation reaction, thereby forming
20 cyclomaltodextrins (or CD) of various sizes.

CGTases are widely distributed and from several different bacterial sources, including *Bacillus*, *Brevibacterium*, *Clostridium*, *Corynebacterium*, *Klebsiella*, *Micrococcus*, *Thermoanaerobacter* and *Thermoanaerobacterium* have been extensively described in the literature. A CGTase produced by *Thermoanaerobacter* sp.
25 has been reported in Norman B E, Jørgensen S T; Denpun Kagaku 1992 39 99-106, and WO 89/03421, and the amino acid sequence has been disclosed in WO 96/33267. The sequence of CGTases from *Thermoanaerobacterium thermosulfurigenes* and from *Bacillus circulans* is available on the Internet (SCOP or PDF home pages) as pdf file 1CIU, and the sequence of a CGTase from *B. circulans* is available as pdf file 1CDG.

30 Tachibana, Y., Journal of Fermentation and Bioengineering, 83 (6), 540-548 (1997) describes the cloning and expression of a CGTase. Variants of CGTases have been described by Kim, Y. H., Biochemistry and Molecular Biology International, 41 (2), 227-234 (1997); Sin K-A, Journal of Biotechnology, 32 (3), 283-288 (1994); D Penninga, Biochemistry, 34 (10), 3368-3376 (1995); and WO 96/33267.

Recently, the tertiary structure of several CGTases have been reported. *Hofman et al.* [*Hofman B E, Bender H, Schultz G E; J. Mol. Biol.* 1989 **209** 793-800] and *Klein & Schulz* [*Klein C, Schulz G E; J. Mol. Biol.* 1991 **217** 737-750] report the tertiary structure of a CGTase derived from *Bacillus circulans* Strain 8, *Kubota et al.* [*Kubota M,*
5 *Matsuura Y, Sakai S and Katsube Y; Denpun Kagaku* 1991 **38** 141-146] report the tertiary structure of a CGTase derived from *Bacillus stearothermophilus* TC-91, *Lawson et al.* [*Lawson C L, van Montfort R, Strokopytov B, Rozeboom H J, Kalk K H, de Vries G E, Penninga D, Dijkhuizen L, and Dijkstra B W; J. Mol. Biol.* 1994 **236** 590-600] report the tertiary structure of a CGTase derived from *Bacillus circulans* Strain 251,
10 *Strokopytov et al.* [*Strokopytov B, Penninga D, Rozeboom H J; Kalk K H, Dijkhuizen L and Dijkstra B W; Biochemistry* 1995 **34** 2234-2240] report the tertiary structure of a CGTase derived from *Bacillus circulans* Strain 251, which CGTase has been complexed with acarbose, an effective CGTase inhibitor, and *Knegt et al.* [*Knegt R M A, Wind R D, Rozeboom H J, Kalk K H, Buitelaar R M, Dijkhuizen L and Dijkstra B*
15 *W; J. Mol. Biol.* 1996 **256** 611-622] report the tertiary structure of a CGTase derived from *Thermoanaerobacterium thermosulfurigenes*.

BRIEF DISCLOSURE OF THE INVENTION

The inventors have modified the amino acid sequence of a maltogenic alpha-amylase to obtain variants with improved properties, based on the three-dimensional
20 structure of the maltogenic alpha-amylase Novamyl. The variants have altered physicochemical properties., e.g. an altered pH optimum, improved thermostability, increased specific activity, an altered cleavage pattern or an increased ability to reduce retrogradation of starch or staling of bread.

Accordingly, the present invention provides a method of constructing a variant
25 of a parent maltogenic alpha-amylase, wherein the variant has at least one altered property as compared to said parent maltogenic alpha-amylase, which method comprises:

i) analyzing the structure of the maltogenic alpha-amylase to identify, on the basis of an evaluation of structural considerations, at least one amino acid residue or at
30 least one structural region of the maltogenic alpha-amylase, which is of relevance for altering said property;

ii) constructing a variant of the maltogenic alpha-amylase, which as compared to the parent, has been modified in the amino acid residue or structural part identified in i) so as to alter said property; and

35 iii) testing the resulting maltogenic alpha-amylase variant for said property.

The property which may be altered by the above methods of the present invention may be, e.g., stability, pH dependent activity, ability to reduce retrogradation

of starch or staling of bread, specific activity, or substrate specificity. Thus, the variant may have, e.g., increased thermostability or higher activity at a lower pH an altered pH optimum, improved thermostability, increased specific activity or increased ability to reduce retrogradation of starch or staling of bread

- 5 In still further aspects the invention relates to variants of a maltogenic alpha-amylase, the DNA encoding such variants and methods of preparing the variants. Finally, the invention relates to the use of the variants for various industrial purposes, in particular baking.

DETAILED DISCLOSURE OF THE INVENTION

10 Maltogenic alpha-amylase

The maltogenic alpha-amylase is an enzyme classified in EC 3.2.1.133. The enzymatic activity does not require a non-reducing end on the substrate and the primary enzymatic activity results in the degradation of amylopectin and amylose to maltose and longer maltodextrins. It is able to hydrolyze amylose and amylopectin to
15 maltose in the alpha-configuration, and is also able to hydrolyze maltotriose as well as cyclodextrin.

A particularly preferred maltogenic alpha-amylase is the amylase cloned from *Bacillus* as described in EP 120 693 (hereinafter referred to as Novamyl). Novamyl has the amino acid sequence set forth in amino acids 1-686 of SEQ ID NO: 1. Novamyl is
20 encoded in the gene harbored in the *Bacillus* strain NCIB 11837 which has the nucleic acid sequence set forth in SEQ ID NO:1. The three-dimensional structure of Novamyl is described below.

In general, a preferred maltogenic alpha-amylase should have one or more of the following properties:

- 25 i) a three dimensional structural homology to Novamyl,
ii) an amino acid sequence having at least 70 % identity to SEQ ID NO: 1, preferably at least 80 % or 90 %, e.g. 95 % or 98 %,
iii) a DNA sequence which hybridizes to the DNA sequence set forth in SEQ ID NO:1 or to the DNA sequence encoding Novamyl harbored in the *Bacillus* strain NCIB
30 11837;
iv) a calcium binding site comprising a coordination equivalent to a backbone carbonyl atom from Asn77, sidechain atom OE2 and OE1 from Glu102, a sidechain atom OD1 from Asp79, a sidechain atom OD1 from Asp76, and a sidechain atom OE1 from Glu101, and one water molecule WAT V21, atom OW0, wherein the positions are
35 as shown in Appendix 1;

v) a sequence of five amino acids corresponding to Pro-Ala-Gly-Phe-Ser in a position equivalent to residues 191-195 in the amino acid sequence shown in SEQ ID NO: 1; and

The structural homology referred to above in i) is based on other sequence
5 homologies, hydrophobic cluster analysis or by reverse threading (Huber, T ; Torda, AE, PROTEIN SCIENCE Vol. 7 , No. 1 pp. 142-149 (1998)) and which by any of these methods is predicted to have the same tertiary structure as Novamyl, wherein the tertiary structure refers to the overall folding or the folding of Domains A, B, and C, more preferably including Domain D, and most preferably including Domain E.
10 Alternatively, a structural alignment between Novamyl and a maltogenic alpha-amylase may be used to identify equivalent positions.

The calcium binding site referred to above in iv) is based on a calcium binding site identified in the three-dimensional structure of Novamyl, and is discussed below in the section "Calcium binding sites."

15 The "equivalent position" referred to above in v) is based on amino acid or DNA sequence alignment or structural homology using methods known in the art.

Three-dimensional structure of maltogenic alpha-amylase

Novamyl was used to elucidate the three-dimensional structure forming the basis for the present invention.

20 The structure of Novamyl was solved in accordance with the principle for x-ray crystallographic methods, for example, as given in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989.

The structural coordinates for the solved crystal structure of Novamyl at 2.2 Å resolution using the isomorphous replacement method are given in standard PDB
25 format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT) as set forth in Appendix 1. It is to be understood that Appendix 1 forms part of the present application. In the context of Appendix 1, the following abbreviations are used: CA refers to calcium ion or alpha-carbon atom of the polypeptide backbone, WAT refers to water or to calcium, MAL refers to maltose, HEX refers to a carbohydrate unit of a
30 substrate analogue, and SUL refers to a sulfate ion.

Amino acid residues of the enzyme are identified herein by their respective one- or three-letter amino acid code.

The structure of said maltogenic alpha-amylase is made up of five globular domains, ordered A, B, C, D and E. The domains can be defined as being residues 1-
35 132 and 204-403 for Domain A, residues 133-203 for Domain B, residues 404-496 for Domain C, residues 497-579 for Domain D, and residues 580-686 for Domain E,

wherein the numbering refers to the amino acid sequence in SEQ ID NO: 1. Features of Domains A, B, and C of particular interest are described below.

Domain A

Domain A is the largest domain and contains the active site which comprises a cluster of three amino acid residues, D329, D228 and E256, spatially arranged at the bottom of a cleft in the surface of the enzyme. The structure of Domain A shows an overall fold in common with the α -amylases for which the structure is known, viz. the (beta/alpha) 8 barrel with eight central beta strands (numbered 1-8) and eight flanking α -helices. The β -barrel is defined by McGregor *op. cit.* The C-terminal end of the beta strand 1 is connected to helix 1 by a loop denoted loop 1 and an identical pattern is found for the other loops, although the loops show some variation in size and some can be quite extensive.

The eight central beta-strands in the (beta/alpha) 8 barrel superimpose reasonably well with the known structures of CGTases. This part of the structure, including the close surroundings of the active site located at the C-terminal end of the beta-strands, shows a high degree of identity with CGTases.

In contrast, the loops connecting the beta-strands and alpha helices display a high degree of variation from the known structures of CGTases. These loops constitute the structural context of the active site, and the majority of the contacts to the substrate is found among residues located in these loops. Distinguishing characteristics such as substrate specificity, substrate binding, pH activity profile, substrate cleavage pattern, and the like, are determined by specific amino acids and the positions they occupy in these loops. In Novamyl Domain A contains two calcium binding sites, one of which is homologous to the calcium binding site in CGTases; the other is unique to Novamyl. The structure of the calcium binding site is discussed further below in the section "Calcium binding sites."

Domain B

Domain B, also referred to as loop 3 of the (beta/alpha) 8 barrel, in comprises amino acid residues 133-203 of the amino acid sequence shown in SEQ ID NO: 1. The structure is partially homologous to the structure of Domain B in CGTases, the most striking difference being the presence of a five amino acid insert corresponding to positions 191-195 in the amino acid sequence shown in SEQ ID NO: 1 which is not found in the CGTases. This insert is spatially positioned close to the active site residues and in close contact to the substrate.

Domain C

Domain C in Novamyl comprises amino acid residues 404-496 of the amino acid sequence shown in SEQ ID NO: 1. Domain C is composed entirely of β -strands which form a single 8-stranded sheet structure that folds back on itself, and thus may be described as a β -sandwich structure. One part of the β -sheet forms the interface to Domain A.

Calcium binding sites

The structure of the maltogenic α -amylase exhibits three calcium-binding sites; that is, three calcium ions are found to be present in the structure. In common with most of the known family 13 structures, one calcium ion, WAT 693 in Appendix 1, is located between the A and B domains. This calcium ion is coordinated by a backbone carbonyl atom from Gln184 and His232, sidechain atoms OD2 and OD1 from Asp198, a sidechain atom OD1 from Asn131, and three water molecules WAT V1, WAT V5 and WAT V8.

A second calcium ion is located in the A domain and is common to CGTases, but not found in α -amylases. The calcium ion WAT 694 is coordinated by a backbone carbonyl atom from Gly48 and Asp23, sidechain atom OD2 from Asp50, a sidechain atom OD1 from Asp21, a sidechain atom OD1 from Asn26, and a sidechain atom OD1 from Asn27, and one water molecule WAT V62.

The third calcium ion is located in the A Domain and is unique to Novamyl. The calcium ion is WAT 692 and the coordination comprises a backbone carbonyl atom from Asn77, sidechain atom OE2 and OE1 from Glu102, a sidechain atom OD1 from Asp79, a sidechain atom OD1 from Asp76, and a sidechain atom OE1 from Glu101, and one water molecule WAT V21.

Substrate Binding Site

Parts of the loop discussed above in the context of domains A and B are of particular interest for substrate interaction and active site reactivity. In particular, in domain A, residues 37-45 in loop 1, residues 261-266 in loop 5, residues 327-330 in loop 7 and residues 370-376 in loop 8; in domain B, residues 135-145 in loop 3, residues 173-180 and 188-196 in loop 3, wherein residue positions correspond to the amino acids in the amino acid sequence in SEQ ID NO: 1.

Without being limited to any theory, it is presently believed that binding between a substrate and an enzyme is supported by favorable interactions found within a sphere of 4 to 6 Å between the substrate molecule and the enzyme, such as hydrogen bonds and/or strong electrostatic interaction. The following residues of

Novamyl (SEQ ID NO: 1), are within a distance of 6 Å of the substrate HEX and thus believed to be involved in interactions with said substrate:

44, 89, 90, 92, 93, 127, 129, 132, 135, 177, 178, 188, 191, 194, 196, 226, 228, 229, 230, 231, 232, 256, 258-261, 288, 328, 329, 371, 372, 373, 376, and 690.

- 5 The following residues of Novamyl are within a distance of 4 Å of the substrate HEX and thus believed to be involved in interactions with said substrate:

90, 92, 93, 129, 132, 177, 188, 189, 190, 191, 196, 226, 228, 229, 231, 232, 256, 258, 259, 260, 261, 328, 329, 372, 376, and 690.

Homology building of Novamyl®

- 10 The structure of the Novamyl® was model built on the structure disclosed in Appendix 1 herein. The structure of other maltogenic alpha-amylases may be built analogously.

A model structure of a maltogenic alpha-amylase can be built using the Homology program or a comparable program, eg., Modeller (both from Molecular
15 Simulations, Inc., San Diego, CA). The principle is to align the sequence of the maltogenic alpha-amylase with the known structure with that of the maltogenic alpha-amylase for which a model structure is to be constructed. The structurally conserved regions can then be built on the basis of consensus sequences. In areas lacking
20 homology, loop structures can be inserted, or sequences can be deleted with subsequent bonding of the necessary residues using, e.g., the program Homology. Subsequent relaxing and optimization of the structure should be done using either Homology or another molecular simulation program, e.g., CHARMM from Molecular Simulations.

Methods for designing novel maltogenic alpha-amylase variants

- 25 In a first aspect, the invention relates to a method of constructing a variant of a parent maltogenic alpha-amylase, wherein said variant has at least one altered property as compared to said parent α -amylase, which method comprises:

i) analyzing the structure of the maltogenic alpha-amylase to identify at least one amino acid or structural region of said α -amylase, which, on the basis of structural
30 or functional considerations, is determined to be of relevance for altering said property of the parent maltogenic alpha-amylase;

ii) constructing a variant of the maltogenic alpha-amylase, which as compared to the parent, has been modified in the amino acid residue or structural region identified in i) has been modified so as to alter said property; and

- 35 iii) testing the resulting variant for said property.

The structural part which is identified in step i) of the method of the invention may be composed of one amino acid residue. However, normally the structural part comprises more than one amino acid residue, typically constituting one of the above parts of the maltogenic alpha-amylase structure such as one of the A, B, C, D or E domains, an interface between any of these domains, a calcium binding site, a loop structure, the substrate binding site, or the like.

The structural or functional considerations may involve an analysis of the relevant structure or structural part and its contemplated impact on the function of the enzyme. For example, an analysis of the functional differences between maltogenic alpha-amylase and the various CGTases may be used for assigning certain properties of Novamyl to certain parts of the Novamyl structure or to contemplate such relationship. For instance, differences in the pattern or structure of loops surrounding the active site may result in differences in access to the active site of the substrate and thus differences in substrate specificity and/or cleavage pattern.

Furthermore, parts of a maltogenic alpha-amylase involved in substrate binding, and thus, for example, substrate specificity and/or cleavage, calcium ion binding, important, for example, for the calcium dependency of the enzyme, and the like, have been identified (*vide infra*).

The modification of an amino acid residue or structural region is typically accomplished by suitable modifications of a DNA sequence encoding the parent enzyme in question. The modification may be substitution, deletion or insertion of an amino acid residue or a structural part.

The property to be modified may be stability (e.g. thermostability), pH dependent activity, substrate specificity, specific activity or ability to reduce retrogradation of starch or staling of bread. Thus, the altered property may be an altered specific activity at a given pH and/or an altered substrate specificity, such as an altered pattern of substrate cleavage or an altered pattern of substrate inhibition.

In step ii) of the method according to the invention the part of the structure to be identified is preferably one which in the folded enzyme is believed to be in contact with the substrate (cf, the disclosure above in the section entitled "Substrate Binding Site") or involved in substrate specificity and/or cleavage pattern, and/or one which is in contact with one of the calcium ions and/or one, which is contributing to the pH or temperature profile of the enzyme, or is otherwise responsible for the properties of the maltogenic alpha-amylase.

Described in the following are specific types of variants which have been designed by use of the method of the invention.

The variants of the invention may comprise additional modifications in addition to the modifications described herein. The variants preferably have an amino acid

having more than 70 % identity with SEQ ID NO: 1, preferably more than 80 %, particularly more than 90 %, especially more than 95 %, e.g. more than 98 %.

Maltogenic alpha-amylase variants with altered pH dependent activity profile

The pH dependent activity profile can be changed by changing the pKa of
5 residues within 10 Å of the active site residues of the maltogenic alpha-amylase. Changing the pKa of the active site residues is achieved, e.g., by changing the electrostatic interaction or hydrophobic interaction between functional groups of amino acid side chains of a given amino acid residue and its close surroundings. To obtain a higher activity at a higher pH, negatively charged residues are placed near a hydrogen
10 donor acid, whereas positively charged residues placed near a nucleophilic acid will result in higher activity at low pH. Also, a decrease in the pKa can be obtained by reducing the accessibility of water or increasing hydrophobicity of the environment.

Thus, another aspect of the present invention relates to a variant of a parent maltogenic alpha-amylase, in which the variant has an altered pH dependent activity
15 profile as compared to the parent, wherein the variant may be obtained by the following method:

i) identifying an amino acid residue within 15 Å from an active site residue of a maltogenic alpha-amylase in the three-dimensional structure of said parent maltogenic alpha-amylase, in particular 10 Å from an active site residue, wherein said amino acid
20 residue is contemplated to be involved in electrostatic or hydrophobic interactions with an active site residue;

ii) substituting, in the structure, said amino acid residue with an amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue, and evaluating the accommodation of the amino acid residue in the
25 structure,

iii) optionally repeating step i) and/or ii) recursively until an amino acid substitution has been identified which is accommodated into the structure,

iv) constructing a maltogenic alpha-amylase variant resulting from steps i) and ii), and optionally iii), and testing the pH dependent enzymatic activity of said variant.

30 In a preferred embodiment, the variant of a maltogenic alpha-amylase having an altered pH dependent activity profile as compared to the parent maltogenic alpha-amylase comprises a modification of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

D127, V129, F188, A229, Y258, V281, F284, T288, N327, M330, G370, N371,
35 and D372,

L71, S72, V74, L75, L78, T80, L81, G83, T84, D85, N86, T87, G88, Y89, H90, G91, T94, R95, D96, F97, I174, S175, N176, D178, D179, R180, Y181, E182, A183, Q184, K186, N187, F188, T189, D190, A192, G193, F194, S195, L196.

In more preferred embodiment, the variant comprises a modification
 5 corresponding to one or more of the following modifications in the amino acid sequence set forth in SEQ ID NO: 1:

D127N/L, V129S/T/G/V, F188E/K/H, A229S/T/G/V, Y258E/D/K/R/F/N, V281L/T, F284K/H/D/E/Y, T288E/K/R, N327D, M330L/F/I/D/E/K, G370N, N371D/E/G/K, and D372N/V,

10 L71I, S72C, V74I, L75N/D/Q/I/V, L78N/I, T80I/L/V/S/N/G, L81I/V/S/T/N/Q/K/H, G83A/S/T/N/Q/E/D/R/H/L, T84S/A/N/D/G, D85A/T/S/N/G, N86Q/E/D/Y/H/K, T87S/I, G88A/S/T, Y89F, H90N/Q/K, G91A/S/T, T94N/D/A/M/V/I, R95K/Q, D96N/V/Q/I, F97Y, I174N/Q/L, S175T/A/N/D, N176S/T/H/Q/P, D178N/Q/E/K/H, D179Y/N/H, R180W, Y181R/F/C/L, E182D, A183S/C/G, Q184E, K186R, N187Q/E/L/F/H/K/V/L,
 15 F188Y/L/I/H/N, T189N/D/A/S/H/Y/G, D190E/Q/H/N/K, A192T/D/E/N/K, G193A/S/T, F194Y, S195N/D/E/R/K/G, L196I.

Similar modifications may be introduced in equivalent positions of other maltogenic alpha-amylases. Variants of particular interest have a combination of one or more of the above with any of the other modifications disclosed herein.

20 **Maltogenic alpha-amylase variants with altered stability**

A variant with improved stability (typically increased stability) may be obtained by stabilization of calcium binding, substitution with proline, substitution of histidine with another amino acid, introduction of an interdomain disulfide bond, removal of a deamidation site, altering a hydrogen bond contact, filling in an internal structural cavity
 25 with one or more amino acids with bulkier side groups, introduction of interdomain interactions, altering charge distribution, helix capping, or introduction of a salt bridge.

Calcium binding

The invention provides a variant of a parent maltogenic alpha-amylase, which has an altered stability due to an altered stabilization of calcium (Ca^{2+}) binding. The
 30 enzyme variant may have altered thermostability or pH dependent stability, or it may have maltogenic alpha-amylase activity in the presence of a lower concentration of calcium ion. It is presently believed that amino acid residues located within 10 Å from a calcium ion are involved in or are of importance for the Ca^{2+} binding capability of the enzyme.

The amino acid residues found within a distance of 10 Å from the Ca²⁺ binding sites of the maltogenic alpha-amylase with the amino acid sequence set forth in SEQ ID NO: 1 were determined as described in Example 2 and are as follows:

16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 35, 36, 40,
5 46, 47, 48, 49, 50, 51, 52, 53, 54, 56, 73, 74, 75, 76, 77, 78, 79, 80, 81, 87, 88, 89, 91,
93, 94, 95, 96, 99, 100, 101, 102, 103, 104, 105, 109, 129, 130, 131, 132, 133, 134,
145, 150, 167, 168, 169, 170, 171, 172, 174, 177, 180, 181, 182, 183, 184, 185, 186,
187, 188, 189, 196, 197, 198, 199, 200, 201, 202, 206, 210, 228, 229, 230, 231, 232,
233, 234, 235, 237, 378, and 637.

10 In order to construct a variant according to this aspect of the invention it is desirable to substitute at least one of the above mentioned amino acid residues, which is determined to be involved in a non-optimal calcium binding, with any other amino acid residue which improves the Ca²⁺ binding affinity of the variant enzyme. Accordingly, another aspect of the invention relates to a method of constructing a
15 variant of a parent maltogenic alpha-amylase wherein said variant has a stabilised Ca²⁺ binding as compared to said parent, which method comprises:

i) identifying an amino acid residue within 10 Å from a Ca²⁺ binding site of a maltogenic alpha-amylase in a model of the three-dimensional structure of said α-amylase which, from structural or functional considerations, is determined to be
20 responsible for a non-optimal calcium ion interaction;

ii) constructing a variant in which said amino acid residue is substituted with another amino acid residue which, from structural or functional considerations, is determined to be important for establishing an altered Ca²⁺ binding affinity; and

iii) testing the Ca²⁺ binding of the resulting maltogenic alpha-amylase variant.

25 Substituting an amino acid residue responsible for non-optimal calcium ion interaction with another residue may alter a calcium ion binding interaction of the enzyme. For instance, the amino acid residue in question may be selected on the basis of one or more of the following objectives:

a) to obtain an improved interaction between a calcium ion and an amino acid
30 residue as identified from the structure of the maltogenic alpha-amylase. For instance, if the amino acid residue in question is exposed to a surrounding solvent, it may be advantageous to increase the shielding of said amino acid residue from the solvent so as to stabilize the interaction between said amino acid residue and a calcium ion. This can be achieved by substituting said residue, or an amino acid residue in the vicinity of
35 said residue contributing to the shielding, with an amino acid residue with a bulkier side group or which otherwise results in an improved shielding effect.

b) to stabilize a calcium binding site, for instance by stabilizing the structure of the maltogenic alpha-amylase, e.g. by stabilizing the contacts between two or more of

the five domains or stabilizing one or more of the individual domains as such. This may, e.g., be achieved by providing for a better coordination to amino acid side chains, which may, e.g., be obtained by substituting an N residue with a D residue and/or a Q residue with an E residue, e.g. within 10 Å, and preferably within 3 or 4 Å, of a calcium binding
5 site.

c) to improve the coordination between the calcium ion and the calcium binding residues, e.g., by improving the interaction between the ion and the coordinating residues or increasing the number of sidechain coordinations by substituting a coordinating water with an amino acid sidechain.

10 d) replace water by a coordinating calcium amino acid residue.

Preferably, the amino acid residue to be modified is located within 8 Å of a Ca^{2+} ion, preferably within 5 Å of a Ca^{2+} ion. The amino acid residues within 8 Å and 5 Å, respectively, may easily be identified by an analogous method used for identifying amino acid residues within 10 Å (cf. Example 2).

15 In a preferred embodiment, the variant of a maltogenic alpha-amylase having an altered Ca^{2+} binding as compared to the parent maltogenic alpha-amylase comprises a substitution of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

D17, A30, S32, R95, H103, N131, Q201, I174, and/or H169,
20 V74, L75, L78, T80, L81, T87, G88, Y89, H90, G91, T94, R95, D96, F97, Y167, F168, H169, H170, N171, G172, D173, I174, S175, N176, D178, D179, R180, Y181, E182, A183, Q184, K186, N187, F188, T189.

In more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions in
25 the amino acid sequence set forth in SEQ ID NO: 1:

D17E/Q, A30M/L/A/V/I/E/Q, S32D/E/N/Q, R95M/L/A/V/I/E/Q, H103Y/N/Q/D/E, N131D, Q201E, I174E/Q, and H169N/D/E/Q

V74I, L75N/D/Q/I/V, L78N/I, T80I/L/V/S/N/G, L81I/V/S/T/N/Q/K/H, T87S/I, G88A/S/T, Y89F, H90N/Q/K, G91A/S/T, T94N/D/A/M/V/I, R95K/Q, D96N/V/Q/I, F97Y,
30 Y167F/R/C, F168Y, H169N/Q/K, H170N/Q/K, N171D/E/Q/H/R/K/G, G172A/T/S, D173N/S/T/Y/R/G, I174N/Q/L, S175T/A/N/D, N176S/T/H/Q/P, D178N/Q/E/K/H, D179Y/N/H, R180W, Y181R/F/C/L, E182D, A183S/C/G, Q184E, K186R, N187Q/E/L/F/H/K/V/L, F188Y/L/I/H/N, T189N/D/A/S/H/Y/G.

In another preferred embodiment of the invention with respect to altering the
35 Ca^{2+} binding of a maltogenic alpha-amylase the partial sequence N28-P29-A30-K31-S32-Y33-G34 as set forth in SEQ ID NO: 1 is modified.

Similar substitutions may be introduced in equivalent positions of other maltogenic alpha-amylases. Modifications of particular interest are any combination of one or more of the above with any of the other modifications disclosed herein.

Other substitutions

- 5 Variants with improved stability of the enzyme can be achieved by improving existing or introducing new interdomain and intradomain contacts. Such improved stability can be achieved by the modifications listed below.

The maltogenic alpha-amylase having the amino acid sequence shown in SEQ ID NO: 1 may be stabilized by the introduction of one or more interdomain disulfide
10 bonds. Accordingly, another preferred embodiment of the present invention relates to a variant of a parent maltogenic alpha-amylase which has improved stability and at least one more interdomain disulfide bridge as compared to said parent, wherein said variant comprises a modification in a position corresponding to at least one of the following pairs of positions in SEQ ID NO: 1:

- 15 G236 + S583, G618 + R272, T252 + V433 and/or A348 + V487.

In a more preferred embodiment, the substitution corresponds to at least one of the following pairs:

G236C + S583C, G618C + R272C, T252C + V433C and/or A348C + V487C.

Another preferred embodiment of the invention relates to a variant of a parent
20 maltogenic alpha-amylase which has an improved stability and an altered interdomain interaction as compared to said parent, wherein said variant comprises a substitution in a position corresponding at least one of the following sets of positions in SEQ ID NO: 1:

- i) F143, F194, L78;
ii) A341, A348, L398, I415, T439, L464, L465;
25 iii) L557;
iv) S240, L268;
v) Q208, L628;
vi) F427, Q500, N507, M508, S573; and
vii) I510, V620.

- 30 In a more preferred embodiment, the substitution corresponds to at least one of the following sets:

- i) F143Y, F194Y, L78Y/F/W/E/Q;
ii) A341S/D/N, A348V/I/L, L398E/Q/N/D, I415E/Q, T439D/E/Q/N, L464D/E,
L465D/E/N/Q/R/K;
35 iii) L557Q/E/N/D;
iv) S240D/E/N/Q, L268D/E/N/Q/R/K;
v) Q208D/E/Q, L628E/Q/N/D;

vi) F427E/Q/R/K/Y, Q500Y, N507Q/E/D, M508K/R/E/Q, S573D/E/N/Q; and/or
vii) I510D/E/N/Q/S, V620D/E/N/Q.

Another preferred embodiment of the invention relates to a variant of a parent maltogenic alpha-amylase which has an improved stability and one or more salt bridges
5 as compared to said parent, wherein said variant comprises a substitution in a position corresponding at least one of the following sets of positions in SEQ ID NO: 1:

N106, N320 and Q624.

In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to the following substitutions in the amino acid
10 sequence set forth in SEQ ID NO: 1:

N106R, N320E/D and/or Q624E.

Another embodiment of the invention relates to a variant of a parent maltogenic alpha-amylase which has an improved stability and wherein said variant comprises a substitution in a position corresponding at least one of the following sets of positions in
15 SEQ ID NO: 1:

K40, V74, S141, T142, F188, N234, K249, D261, L268, V279, N342, G397, A403, K425, S442, S479, S493, T494, S495, A496, S497, A498, Q500, K520, A555 and N595.

In a more preferred embodiment, the variant of a maltogenic alpha-amylase
20 comprises a substitution corresponding to one or more of the following substitutions with proline in the amino acid sequence set forth in SEQ ID NO: 1:

V74P, S141P, N234P, K249P, L268P, V279P, N342P, G397P, A403P, S442P, S479P, S493P, T494P, S495P, A496P, S497P, A498P, Q500P, and/or A555P.

Other preferred substitutions are K40R, T142A, F188I/L, D261G, K425E,
25 K520R, and/or N595I.

Analogously, it may be preferred that one or more histidine residues present in the parent maltogenic alpha-amylase is or are substituted with a non-histidine residues such as Y, V, I, L, F, M, E, Q, N, or D. Accordingly, in another preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution of an amino acid
30 residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

H103, H220, and H344

In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions in
35 the amino acid sequence set forth in SEQ ID NO: 1:

H103Y/V/I/L/F/Y, H220Y/L/M, and H344E/Q/N/D/Y.

It may be preferred that one or more asparagine or glutamine residues present in the parent maltogenic alpha-amylase is or are substituted with a residue lacking the

amide on the side chain. Accordingly, in another preferred embodiment, the variant of a Novamyl-like comprises a substitution of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

Q13, N26, N77, N86, N99, Q119, N120, N131, N152, N171, N176, N187,
 5 Q201, N203, N234, Q247, N266, N275, N276, N280, N287, Q299, N320, N327, N342,
 Q365, N371, N375, N401, N436, N454, N468, N474, Q500, N507, N513, Q526, N575,
 Q581, N621, Q624 and N664.

In more preferred embodiment, the variant of a maltogenic alpha-amylase comprises a substitution corresponding to one or more of the following substitutions in
 10 the amino acid sequence set forth in SEQ ID NO: 1:

Q13S/T/A/V/L/I/F/M, N26S/T/A/V/L/I, N77S/T/A/V/L/I, N86S/T/A/V/L/I,
 N99T/S/V/L, Q119T/S, N120S/T/A/V/L/I, N131S/T/A/V/L/I, N152T/S/V/L, N171Y/D/S/T,
 N176S/T/A/V/L/I, N187S/T/A/V/L/I, Q201S/T/A/V/L/I/F/M, N203D/S/T/A/V/L/I,
 N234S/T/A/V/L/I, Q247S/T/A/V/L/I/F/M, N266S/T/A/V/L/I, N275S/T/A/V/L/I,
 15 N276S/T/A/V/L/I, N280S/T/A/V/L/I, N287S/T/A/V/L/I, Q299L/T/S, N320S/T/A/V/L/I,
 N327S/T/A/V/L/I, N342S/T/A/V/L/I, Q365S/T/A/V/L/I, N371S/T/A/V/L/I, N375S/T/A/V/L/I,
 N401S/T/A/V/L/I, N436S/T/A/V/L/I, N454D/S/T/A/V/L/I, N468D/S/T/A/V/L/I,
 N474D/S/T/A/V/L/I, Q500S/T/A/V/L/I/F/M, N507S/T/A/V/L/I, N513S/T/A/V/L/I, Q526
 D/S/T/A/V/L/I, N575S/T/A/V/L/I, Q581S/T/A/V/L/I/F/M, N621S/T/A/V/L/I
 20 Q624S/T/A/V/L/I/F/M and N664D/S/T/A/V/L/I.

Another embodiment of the invention relates to a variant of a parent maltogenic alpha-amylase which has improved stability and improved hydrogen bond contacts as compared to said parent, wherein said variant comprises a modification in a position corresponding to one or more of the following positions in SEQ ID NO: 1:

25 I16, L35, M45, P73, D76, D79, A192, I100, A148, A163+G172, L268, V281,
 D285, L321, F297, N305, K316, S573, A341, M378, A381, F389, A483, A486, I510,
 A564, F586, K589, F636, K645, A629, and/or T681.

In a preferred embodiment, the modification corresponds to one or more of the following:

30 I16T/D/N, L35Q, M45K, P73Q, D76E, D79E/Y, A192S/D/N, I100T/S/D/N/E/Q,
 A148D/N/E/Q/S/T/R/K, A163Y+G172S/D/N, L268R/K, V281/Q, D285R/K, L321Q,
 F297N/D/Q/E, N305K/R, K316N/D, S573N/D, A341R/K, M378R/K, A381S/D/N, F389Y,
 A483S/D/N, A486Q/E, I510R/K, A564S/D/N, F586S/D/N, K589S/D/Q/N, F636Y,
 K645T, A629N/D/E/Q, and/or T681D/N/E/Q/S.

35 Similar substitutions may be introduced in equivalent positions of other maltogenic alpha-amylases. Substitutions of particular interest are any combination of one or more of the above with any of the other modifications disclosed herein.

Before actually constructing a maltogenic alpha-amylase variant to achieve any of the above objectives, it may be convenient to evaluate whether or not the contemplated amino acid modification can be accommodated into the maltogenic alpha-amylase structure, e.g. into a model of the three-dimensional structure of the parent maltogenic alpha-amylase.

Maltogenic alpha-amylase variants with altered thermostability and/or altered temperature dependent activity profile

The invention further relates to a variant of a parent maltogenic alpha-amylase, which results from substitution, deletion or insertion of one or more amino acid residues so as to obtain a variant having an altered thermostability or temperature dependent activity profile.

The structure of the maltogenic alpha-amylase contains a number of unique internal cavities which may contain water and a number of crevices. In order to increase the thermostability of the polypeptide it may be desirable to reduce the number or size of cavities and crevices, e.g., by introducing one or more hydrophobic contacts, preferably achieved by introducing amino acids with bulkier side groups in the vicinity or surroundings of the cavity. For instance, the amino acid residues to be modified are those which are involved in the formation of the cavity.

Accordingly, in a further aspect the present invention relates to a method of increasing the thermostability and/or altering the temperature dependent activity profile of a parent maltogenic alpha-amylase, which method comprises:

- i) identifying an internal cavity or a crevice of the parent maltogenic alpha-amylase in the three-dimensional structure of said polypeptide;
- ii) substituting, in the structure, one or more amino acid residues in the neighbourhood of the cavity or crevice identified in step i) with another amino acid residue which, from structural or functional considerations, is determined to increase the hydrophobic interaction and to fill out or reduce the size of the cavity or crevice; and
- iii) constructing a variant of the parent maltogenic alpha-amylase resulting from step ii) and testing the thermostability and/or temperature dependent activity of the variant.

The structure identified in Appendix 1 may be used for identifying the cavity or crevice of the parent maltogenic alpha-amylase.

It will be understood that the cavity or crevice is identified by the amino acid residues surrounding said cavity or crevice, and that modification of said amino acid residues are of importance for filling or reducing the size of said cavity or crevice. Preferably, the modification is a substitution with a bulkier amino acid residue, i.e. one with a greater side chain volume. For example, all the amino acids are bulkier than Gly,

whereas Tyr and Trp are bulkier than Phe. The particular amino acid residues referred to below are those which in a crystal structure have been found to flank the cavity or crevice in question.

In a preferred embodiment, the variant of a maltogenic alpha-amylase, in order to fill, either completely or partly, cavities located internally in the structure, comprises a substitution of an amino acid residue corresponding to one or more of the following residues of the amino acid sequence set forth in SEQ ID NO: 1:

L51, L75, L78, G88, G91, T94, V114, I125, V126, T134, G157, L217, S235, G236, V254, V279, V281, L286, V289, I290, V308, L321, I325, D326, L343, F349, S353, I359, I405, L448, Q449, L452, I470, G509, V515, S583, G625, L627, L628 and A670.

L71, S72, V74, L75, L78, T80, L81, G83, T84, D85, N86, T87, G88, Y89, H90, G91, T94, R95, D96, F97, Y167, F168, H169, H170, N171, G172, D173, I174, S175, N176, D178, D179, R180, Y181, E182, A183, Q184, K186, N187, F188, T189, D190, A192, G193, F194, S195, L196.

In a more preferred embodiment, the variant of a maltogenic alpha-amylase comprises one or more substitutions corresponding to the following substitutions in the amino acid sequence set forth in SEQ ID NO: 1:

L217 in combination with L75 (e.g. L217F/Y in combination with L75F/Y), L51W, L75F/Y, L78I, G88A/V/T, G91T/S/V/N, T94V/I/L, V114V/I/L, I125L/M/F/Y/W, V126I/L, T134V/I/L/M/F/Y/W, G157A/V/I/L, L217V/I/M/F/Y/W, S235I/L/M/F/Y/W, G236A/V/I/L/M/F/Y/W, V254I/L/M/F/Y/W, V279M/I/L/F, V281I/L/M/F/Y/W, L286F, V289I/L/R, I290M/L/F, V308I/L/M/F/Y/W, L321I/M/F/Y/W, I325L/M/F/Y/W, D326E/Q, L343M/F/Y/W, F349W/Y, S353V/I/L, I359L/M/F/Y/W, I405M/L/Y/F/W, L448Y, Q449Y, L452M/Y/F/W, I470M/L/F, G509A/V/I/L/M/S/T/D/N, V515I/L, S583V/I/L/V, G625A/V/I/L/M/F/Y/W, L627M/F/Y, L628M/I/F/Y/W and A670V/I/L/M/F/Y/W,

L71I, S72C, V74I, L75N/D/Q/I/V, L78N/I, T80I/L/V/S/N/G, L81I/V/S/T/N/Q/K/H, G83A/S/T/N/Q/E/D/R/H/L, T84S/A/N/D/G, D85A/T/S/N/G, N86Q/E/D/Y/H/K, T87S/I, G88A/S/T, Y89F, H90N/Q/K, G91A/S/T, T94N/D/A/M/V/I, R95K/Q, D96N/V/Q/I, F97Y, Y167F/R/C, F168Y, H169N/Q/K, H170N/Q/K, N171D/E/Q/H/R/K/G, G172A/T/S, D173N/S/T/Y/R/G, I174N/Q/L, S175T/A/N/D, N176S/T/H/Q/P, D178N/Q/E/K/H, D179Y/N/H, R180W, Y181R/F/C/L, E182D, A183S/C/G, Q184E, K186R, N187Q/E/L/F/H/K/V/L, F188Y/L/I/H/N, T189N/D/A/S/H/Y/G, D190E/Q/H/N/K, A192T/D/E/N/K, G193A/S/T, F194Y, S195N/D/E/R/K/G, L196I.

Similar substitutions may be introduced in equivalent positions of other maltogenic alpha-amylases. Variants of particular interest have a combination of one or more of the above with any of the other modifications disclosed herein.

Maltogenic alpha-amylase variants with an altered cleavage pattern

One aim of the present invention is to change the degradation characteristics of a maltogenic alpha-amylase. Thus, Novamyl hydrolyzes starch to form predominantly maltose (G2) and a small amount of glucose (G1), but virtually no higher
5 oligosaccharides (G3+). It may be desirable to change this cleavage pattern, e.g. so as to form higher amounts of higher oligosaccharides, such as maltotriose (G3), maltotetraose (G4) and maltopentaose (G5).

A variant of a parent maltogenic alpha-amylase in which the substrate cleavage pattern is altered as compared to said parent may be constructed by a method which
10 comprises:

- i) identifying the substrate binding area of the parent maltogenic alpha-amylase in a model of the three-dimensional structure, e.g. within a sphere of 4 Å from the substrate binding site as defined in the section above entitled "Substrate Binding Site";
- ii) substituting in the model one or more amino acid residues of the substrate
15 binding area of the cleft identified in i) which is or are believed to be responsible for the cleavage pattern of the parent with another amino acid residue which from structural or functional considerations is believed to result in an altered substrate cleavage pattern, or deleting one or more amino acid residues of the substrate binding area contemplated to introduce favorable interactions to the substrate or adding one or more
20 amino acid residues to the substrate binding area contemplated to introduce favorable interactions to the substrate; and
- iii) constructing a maltogenic alpha-amylase variant resulting from step ii) and testing the substrate cleavage pattern of the variant.

Accordingly, another aspect of the invention relates to a variant of a parent
25 maltogenic alpha-amylase which has an altered substrate binding site as compared to said parent, which variant comprises a modification in a position corresponding to one or both of the following positions in SEQ ID NO: 1:

V281 and/or A629.

In a preferred embodiment, the variant comprises a modification corresponding
30 to:

V281Q and/or A629N/D/E/Q.

Similar modifications may be introduced in equivalent positions of other maltogenic alpha-amylases. Substitutions of particular interest are any combination of one or both of the above with any of the other modifications disclosed herein.

Maltogenic alpha-amylase variants with improved ability to reduce retrogradation of starch and/or staling of bread

The invention provides maltogenic alpha-amylase variants having improved ability to reduce the retrogradation of starch and/or the staling of bread. Preferred
5 variants comprise a modification at one or more positions corresponding to the following amino acid residues in SEQ ID NO: 1:

A30, K40, N115, T142, F188, T189, P191, A192, G193, F194, S195, D261, N327, K425, K520 and N595.

In a more preferred embodiment, the variant comprises one or more
10 modifications corresponding to the following in SEQ ID NO: 1:

A30D, K40R, N115D, T142A, F188L, T189Y, Δ (191-195), D261G, D261G, N327S, K425E, K520R and N595I.

Determination of residues within 10Å from calcium ions

The coordinates of Appendix 1 are read into the INSIGHT program (BIOSYM
15 Technologies). The spatial coordinates are presented showing the bonds between the atoms. The ions are presented as well as the water atoms. The part of the program package for creating subsets was used to create a 10 Å subset around the calcium ions in the structure by using the command ZONE. All residues identified as having an atom within the designated 10 Å distance from a calcium ion are compiled and listed by using
20 the command LIST MOLECULE. By giving the ions the name "VAT CA" in the coordinate file, a 10 Å sphere around all atoms called "VAT CA" is compiled. The specific residues identified in this manner are given further above in the section entitled "Calcium binding".

25 Determination of cavities

The solved structure of Novamyl with the structural coordinates set forth in Appendix 1 reveals many internal crevices and cavities. When analysing for such cavities the Connolly program is normally used (Lee, B. and Richards, F.M. (1971) J. Mol. Biol. 55:379-400). The program uses a probe with radius to search the external
30 and internal surface of the protein. The smallest crevice observable in this way has the probe radius.

To analyse the solved structure a modified version of the Connolly program included in the program of INSIGHT was used. In the first step, the water molecules and the ions were removed by unmerging these atoms from the solved structure. By
35 using the command MOLECULE SURFACE SOLVENT the solvent accessible surface area was calculated for all atoms and residues using a probe radius of 1.4 Å, and

displayed graphically together with the model of the solved structure. The internal cavities are then seen as dot surfaces with no connections to the external surface.

Suggestions for specific modifications to fill out the cavities are given above in the section entitled "Variants with altered thermostability and/or altered temperature dependent activity profile"). By using the homology built structures or/and comparisons based on sequence alignment, mutations for homologous structures of maltogenic alpha-amylases can be made.

Nomenclature for amino acid modifications

10 The nomenclature used herein for defining mutations is essentially as described in WO 92/05249. Thus, F188H indicates a substitution of the amino acid F (Phe) in position 188 with the amino acid H (His). V129S/T/G/V indicates a substitution of V129 with S, T, G or V. Δ (191-195) or Δ (191-195) indicates a deletion of amino acids in positions 191-195. 192-A-193 indicates an insertion of A between amino acids
15 192 and 193.

Polypeptide sequence identity

For purposes of the present invention, the degree of identity may be suitably determined according to the method described in Needleman, S.B. and Wunsch, C.D., (1970), Journal of Molecular Biology, 48, 443-45, with the following settings for
20 polypeptide sequence comparison: GAP creation penalty of 3.0 and GAP extension penalty of 0.1. The determination may be done by means of a computer program known such as GAP provided in the GCG program package (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711).

25 The variants of the invention have an amino acid identity with amino acids 1-686 of SEQ ID NO: 1 of at least 70 %, preferably at least 80 %, e.g. at least 90 %, particularly at least 95 % or at least 98 %.

Hybridization

Suitable experimental conditions for determining hybridization between a
30 nucleotide probe and a homologous DNA or RNA sequence involves presoaking of the filter containing the DNA fragments or RNA to hybridize in 5x SSC (sodium chloride/sodium citrate, Sambrook, et al., 1989) for 10 min, and prehybridization of the filter in a solution of 5x SSC, 5x Denhardt's solution (Sambrook, et al., 1989), 0.5% SDS and 100 μ g/ml of denatured sonicated salmon sperm DNA (Sambrook, et al.,
35 1989), followed by hybridization in the same solution containing a random-primed

(Feinberg, A. P. and Vogelstein, B. (1983) *Anal. Biochem.* 132:6-13), ^{32}P -dCTP-labeled (specific activity $> 1 \times 10^8$ cpm/ μg) probe for 12 hours at ca. 45°C. The filter is then washed twice for 30 minutes in 2x SSC, 0.5% SDS at least 55°C (low stringency), preferably at least 60°C (medium stringency), more preferably at least 65°C
5 (medium/high stringency), more preferably at least 70°C (high stringency), even more preferably at least 75°C (very high stringency).

Molecules which hybridize to the oligonucleotide probe under these conditions are detected by exposure to x-ray film.

Methods of preparing variants of maltogenic alpha-amylases

10 Cloning a DNA sequence encoding a Novamyl-like polypeptide

The DNA sequence encoding a parent maltogenic alpha-amylase may be isolated from any cell or microorganism producing the maltogenic alpha-amylase in question, using various methods well known in the art, for example, from the *Bacillus* strain NCIB 11837.

15 First, a genomic DNA and/or cDNA library should be constructed using chromosomal DNA or messenger RNA from the organism that produces the maltogenic alpha-amylase to be studied. Then, if the amino acid sequence of the α -amylase is known, homologous, labelled oligonucleotide probes may be synthesised and used to identify maltogenic alpha-amylase-encoding clones from a genomic library prepared
20 from the organism in question. Alternatively, a labelled oligonucleotide probe containing sequences homologous to a known α -amylase gene could be used as a probe to identify maltogenic alpha-amylase-encoding clones, using hybridization and washing conditions of lower stringency.

Another method for identifying maltogenic alpha-amylase-encoding clones
25 involves inserting fragments of genomic DNA into an expression vector, such as a plasmid, transforming α -amylase negative bacteria with the resulting genomic DNA library, and then plating the transformed bacteria onto agar containing a substrate for maltogenic alpha-amylase, thereby allowing clones expressing maltogenic alpha-amylase activity to be identified.

30 Alternatively, the DNA sequence encoding the enzyme may be prepared synthetically by established standard methods, e.g. the phosphoroamidite method described by S.L. Beaucage and M.H. Caruthers (1981) or the method described by Matthes et al. (1984). In the phosphoroamidite method, oligonucleotides are synthesized, e.g. in an automatic DNA synthesizer, purified, annealed, ligated and cloned
35 in appropriate vectors.

Finally, the DNA sequence may be of mixed genomic and synthetic origin, mixed synthetic and cDNA origin or mixed genomic and cDNA origin, prepared by ligating fragments of synthetic, genomic or cDNA origin, wherein the fragments correspond to various parts of the entire DNA sequence, in accordance with techniques well known in the art. The DNA sequence may also be prepared by polymerase chain reaction (PCR) using specific primers, for instance as described in US 4,683,202 or R.K. Saiki et al. (1988).

Site-directed Mutagenesis

Once a maltogenic alpha-amylase-encoding DNA sequence has been isolated, and desirable sites for modification identified, modifications may be introduced using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired modification sites; mutant nucleotides are inserted during oligonucleotide synthesis. In a specific method, a single-stranded gap of DNA, bridging the maltogenic alpha-amylase-encoding sequence, is created in a vector carrying the maltogenic alpha-amylase gene. Then the synthetic nucleotide, bearing the desired modification, is annealed to a homologous portion of the single-stranded DNA. The remaining gap is then filled in with DNA polymerase I (Klenow fragment) and the construct is ligated using T4 ligase. A specific example of this method is described in Morinaga et al. (1984). US 4,760,025 discloses the introduction of oligonucleotides encoding multiple modifications by performing minor alterations of the cassette. However, an even greater variety of modifications can be introduced at any one time by the Morinaga method because a multitude of oligonucleotides, of various lengths, can be introduced.

Another method of introducing modifications into a maltogenic alpha-amylase-encoding DNA sequences is described in Nelson and Long (1989). It involves a 3-step generation of a PCR fragment containing the desired modification introduced by using a chemically synthesized DNA strand as one of the primers in the PCR reactions. From the PCR-generated fragment, a DNA fragment carrying the modification may be isolated by cleavage with restriction endonucleases and reinserted into an expression plasmid.

Random Mutagenesis

Random mutagenesis is suitably performed either as localised or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

The random mutagenesis of a DNA sequence encoding a parent maltogenic alpha-amylase may be conveniently performed by use of any method known in the art.

In relation to the above, a further aspect of the present invention relates to a method for generating a variant of a parent Novamyl-like α -amylase, wherein the variant exhibits increased stability at low pH and at low calcium concentration relative to the parent, the method comprising:

- 5 (a) subjecting a DNA sequence encoding the parent Novamyl-like α -amylase to random mutagenesis,
- (b) expressing the mutated DNA sequence obtained in step (a) in a host cell, and
- (c) screening for host cells expressing a Novamyl-like α -amylase variant which
- 10 has an altered property relative to the parent Novamyl-like α -amylase.

Step (a) of the above method of the invention is preferably performed using doped primers, as described in the working examples herein (*vide infra*).

For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by

- 15 subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents. The mutagenizing agent may, e.g., be one which induces transitions, transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present

- 20 purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues. When such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the
- 25 mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleotide at the positions which are to be changed. The

- 30 doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide can be incorporated into the DNA encoding the maltogenic alpha-amylase enzyme by any published technique, using e.g. PCR, LCR or any DNA polymerase and ligase as deemed appropriate.

Preferably, the doping is carried out using "constant random doping", in which

- 35 the percentage of wild-type and modification in each position is predefined. Furthermore, the doping may be directed toward a preference for the introduction of certain nucleotides, and thereby a preference for the introduction of one or more specific amino acid residues. The doping may be made, e.g., so as to allow for the

introduction of 90% wild type and 10% modifications in each position. An additional consideration in the choice of a doping scheme is based on genetic as well as protein-structural constraints. The doping scheme may be made by using the DOPE program which, *inter alia*, ensures that introduction of stop codons is avoided.

5 When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent maltogenic alpha-amylase enzyme is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., Technique, Vol.1, 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., Molec. Gen. Genet., 133, 1974, pp. 10 179-191), *S. cerevisiae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the maltogenic alpha-amylase by, e.g., transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated plasmid from the mutator strain. The mutated plasmid may be subsequently transformed into the expression organism.

15 The DNA sequence to be mutagenized may be conveniently present in a genomic or cDNA library prepared from an organism expressing the parent maltogenic alpha-amylase. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenising agent. The DNA to be mutagenized may also be 20 present in a host cell either by being integrated in the genome of said cell or by being present on a vector harbored in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

In some cases it may be convenient to amplify the mutated DNA sequence 25 prior to performing the expression step b) or the screening step c). Such amplification may be performed in accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

Subsequent to the incubation with or exposure to the mutagenising agent, the 30 mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the 35 following: gram positive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus*

megaterium, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gram negative bacteria such as *E. coli*.

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

5 Localized random mutagenesis

The random mutagenesis may be advantageously localised to a part of the parent maltogenic alpha-amylase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant
10 having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

The localized, or region-specific, random mutagenesis is conveniently performed by use of PCR generated mutagenesis techniques as described above or
15 any other suitable technique known in the art. Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g., by insertion into a suitable vector, and said part may be subsequently subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

For region-specific random mutagenesis with a view to improving the stability of
20 calcium binding of a parent maltogenic alpha-amylase, codon positions corresponding to the following amino acid residues from the amino acid sequence set forth in SEQ ID NO: 1 may appropriately be targeted:

Residues:Regions:

16-33, 35-36, 40: 16-40
25 46-54, 56: 46-56
73-81: 73-81
87-89, 91, 93-96, 99-105, 109: 87-109
129-134, (145, 150): 129-134
167-172, 174, 177, 180-189: 167-189
30 196-202, 206-210: 196-210
228-235, 237: 228-237
378
637

With a view to achieving improved binding of a substrate, i.e., improved binding
35 of a carbohydrate species, such as amylose or amylopectin, by a maltogenic alpha-amylase variant with a modified, e.g. higher, substrate specificity and/or a modified, e.g. higher, specificity with respect to cleavage, i.e. hydrolysis, of the substrate, it appears

that the following codon positions in the following regions of the amino acid sequence shown in SEQ ID NO: 1, may particularly appropriately be targeted for modification by region-specific mutagenesis:

70-97, 127-143, 174-198, 226-233, 255-270, 282-292, 324-331, 370-376.

- 5 For region-specific random mutagenesis with a view to altering the substrate specificity and/or the pH dependent activity profile, the following regions of SEQ ID NO: 1 may be targeted: 70-97, 174-198.

The following regions may be targeted with a view to improving the thermostability: 70-109, 167-200.

10 General method for random mutagenesis by use of the DOPE program

The random mutagenesis may be carried out by the following steps:

1. Select regions of interest for modification in the parent enzyme
2. Decide on mutation sites and nonmutated sites in the selected region
3. Decide on which kind of mutations should be carried out, e.g. with respect to
- 15 the desired stability and/or performance of the variant to be constructed
4. Select structurally reasonable mutations
5. Adjust the residues selected by step 3 with regard to step 4.
6. Analyse by use of a suitable dope algorithm the nucleotide distribution.
7. If necessary, adjust the wanted residues to genetic code realism, e.g. taking
- 20 into account constraints resulting from the genetic code, e.g. in order to avoid introduction of stop codons; the skilled person will be aware that some codon combinations cannot be used in practice and will need to be adapted
8. Make primers
9. Perform random mutagenesis by use of the primers
- 25 10. Select resulting α -amylase variants by screening for the desired improved properties.

Suitable dope algorithms for use in step 6 are well known in the art. One such algorithm is described by Tomandl, D. et al., 1997, Journal of Computer-Aided Molecular Design 11:29-38. Another algorithm is DOPE (Jensen, LJ, Andersen, KV, Svendsen, A, and Kretzschmar, T (1998) Nucleic Acids Research 26:697-702).

Expression of maltogenic alpha-amylase variants

The construction of the variant of interest is accomplished by cultivating a microorganism comprising a DNA sequence encoding the variant under conditions

35 which are conducive for producing the variant, and optionally subsequently recovering the variant from the resulting culture broth. This is described in detail further below.

According to the invention, a DNA sequence encoding the variant produced by methods described above, or by any alternative methods known in the art, can be expressed, in the form of a protein or polypeptide, using an expression vector which typically includes control sequences encoding a promoter, operator, ribosome binding
5 site, translation initiation signal, and, optionally, a repressor gene or various activator genes.

The recombinant expression vector carrying the DNA sequence encoding an maltogenic alpha-amylase variant of the invention may be any vector which may conveniently be subjected to recombinant DNA procedures, and the choice of vector
10 will often depend on the host cell into which it is to be introduced. Thus, the vector may be an autonomously replicating vector, i.e. a vector which exists as an extrachromosomal entity, the replication of which is independent of chromosomal replication, e.g. a plasmid, a bacteriophage or an extrachromosomal element, minichromosome or an artificial chromosome. Alternatively, the vector may be one which, when introduced into
15 a host cell, is integrated into the host cell genome and replicated together with the chromosome(s) into which it has been integrated.

In the vector, the DNA sequence should be operably connected to a suitable promoter sequence. The promoter may be any DNA sequence which shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell. Examples of suitable promoters for directing the transcription of the DNA sequence encoding a maltogenic alpha-amylase variant of the invention, especially in a bacterial host, are the promoter of the *lac* operon of *E.coli*, the *Streptomyces coelicolor* agarase gene *dagA* promoters, the promoters of the *Bacillus licheniformis* α -amylase gene (*amyL*), the promoters of
25 the *Bacillus stearothermophilus* maltogenic amylase gene (*amyM*), the promoters of the *Bacillus amyloliquefaciens* α -amylase (*amyQ*), the promoters of the *Bacillus subtilis* *xylA* and *xylB* genes, etc. For transcription in a fungal host, examples of useful promoters are those derived from the gene encoding *A. oryzae* TAKA amylase, *Rhizomucor miehei* aspartic proteinase, *A. niger* neutral α -amylase, *A. niger* acid stable α -amylase,
30 *A. niger* glucoamylase, *Rhizomucor miehei* lipase, *A. oryzae* alkaline protease, *A. oryzae* triose phosphate isomerase or *A. nidulans* acetamidase.

The expression vector of the invention may also comprise a suitable transcription terminator and, in eukaryotes, polyadenylation sequences operably connected to the DNA sequence encoding the maltogenic alpha-amylase variant of the
35 invention. Termination and polyadenylation sequences may suitably be derived from the same sources as the promoter.

The vector may further comprise a DNA sequence enabling the vector to replicate in the host cell in question. Examples of such sequences are the origins of replication of plasmids pUC19, pACYC177, pUB110, pE194, pAMB1 and pIJ702.

The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, such as the *dal* genes from *B. subtilis* or *B. licheniformis*, or one which confers antibiotic resistance such as ampicillin, kanamycin, chloramphenicol or tetracycline resistance. Furthermore, the vector may comprise *Aspergillus* selection markers such as *amdS*, *argB*, *niaD* and *sC*, a marker giving rise to hygromycin resistance, or the selection may be accomplished by co-transformation, e.g. as described in WO 91/17243.

While intracellular expression may be advantageous in some respects, e.g. when using certain bacteria as host cells, it is generally preferred that the expression is extracellular. In general, the *Bacillus* α -amylases mentioned herein comprise a preregion permitting secretion of the expressed protease into the culture medium. If desirable, this preregion may be replaced by a different preregion or signal sequence, conveniently accomplished by substitution of the DNA sequences encoding the respective preregions.

The procedures used to ligate the DNA construct of the invention encoding maltogenic alpha-amylase variant, the promoter, terminator and other elements, respectively, and to insert them into suitable vectors containing the information necessary for replication, are well known to persons skilled in the art (cf., for instance, Sambrook et al. (1989)).

The cell of the invention, either comprising a DNA construct or an expression vector of the invention as defined above, is advantageously used as a host cell in the recombinant production of a maltogenic alpha-amylase variant of the invention. The cell may be transformed with the DNA construct of the invention encoding the variant, conveniently by integrating the DNA construct (in one or more copies) in the host chromosome. This integration is generally considered to be an advantage as the DNA sequence is more likely to be stably maintained in the cell. Integration of the DNA constructs into the host chromosome may be performed according to conventional methods, e.g. by homologous or heterologous recombination. Alternatively, the cell may be transformed with an expression vector as described above in connection with the different types of host cells.

The cell of the invention may be a cell of a higher organism such as a mammal or an insect, but is preferably a microbial cell, e.g. a bacterial or a fungal (including yeast) cell.

Examples of suitable bacteria are gram positive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermo-*

philus, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, or *Streptomyces lividans* or *Streptomyces murinus*, or gram negative bacteria such as *E.coli*. The transformation of the bacteria may, for instance, be effected by protoplast transformation or
5 by using competent cells in a manner known *per se*.

The yeast organism may favourably be selected from a species of *Saccharomyces* or *Schizosaccharomyces*, e.g. *Saccharomyces cerevisiae*. The filamentous fungus may advantageously belong to a species of *Aspergillus*, e.g. *Aspergillus oryzae* or *Aspergillus niger*. Fungal cells may be transformed by a process
10 involving protoplast formation and transformation of the protoplasts followed by regeneration of the cell wall in a manner known *per se*. A suitable procedure for transformation of *Aspergillus* host cells is described in EP 238 023.

In a yet further aspect, the present invention relates to a method of producing a maltogenic alpha-amylase variant of the invention, which method comprises cultivating
15 a host cell as described above under conditions conducive to the production of the variant and recovering the variant from the cells and/or culture medium.

The medium used to cultivate the cells may be any conventional medium suitable for growing the host cell in question and obtaining expression of the maltogenic alpha-amylase variant of the invention. Suitable media are available from commercial
20 suppliers or may be prepared according to published recipes (e.g. as described in catalogues of the American Type Culture Collection).

The maltogenic alpha-amylase variant secreted from the host cells may conveniently be recovered from the culture medium by well-known procedures, including separating the cells from the medium by centrifugation or filtration, and precipitating
25 proteinaceous components of the medium by means of a salt such as ammonium sulfate, followed by the use of chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

Testing of maltogenic alpha-amylase variants

Maltogenic alpha-amylase variants produced by any of the methods described
30 above may be tested, either prior to or after purification, for amylolytic activity in a screening assay which measures the ability of the variant to degrade starch. The screening in step 10 in the above-mentioned random mutagenesis method of the invention may be conveniently performed by use of a filter assay based on the following procedure: A microorganism capable of expressing the mutated maltogenic alpha-
35 amylase of interest is incubated on a suitable medium and under suitable conditions for secretion of the enzyme, the medium being covered with two filters comprising a protein-binding filter placed under a second filter exhibiting a low protein binding

capability. The microorganism is grown on the second, top filter. Subsequent to the incubation, the bottom protein-binding filter comprising enzymes secreted from the microorganism is separated from the second filter comprising the microorganism. The protein-binding filter is then subjected to screening for the desired enzymatic activity, and the corresponding microbial colonies present on the second filter are identified. The first filter used for binding the enzymatic activity may be any protein-binding filter, e.g., nylon or nitrocellulose. The second filter carrying the colonies of the expression organism may be any filter that has no or low affinity for binding proteins, e.g., cellulose acetate or Durapore™.

Screening consists of treating the first filter to which the secreted protein is bound with a substrate that allows detection of the α -amylase activity. The enzymatic activity may be detected by a dye, fluorescence, precipitation, pH indicator, IR-absorbance or any other known technique for detection of enzymatic activity. The detecting compound may be immobilized by any immobilizing agent e.g. agarose, agar, gelatine, polyacrylamide, starch, filter paper, cloth; or any combination of immobilizing agents. For example, α -amylase activity can be detected by Cibacron Red labelled amylopectin, which is immobilized in agarose. α -amylase activity on this substrate produces zones on the plate with reduced red color intensity.

To screen for variants with increased stability, the filter with bound maltogenic alpha-amylase variants can be pretreated prior to the detection step described above to inactivate variants that do not have improved stability relative to the parent maltogenic alpha-amylase. This inactivation step may consist of, but is not limited to, incubation at elevated temperatures in the presence of a buffered solution at any pH from pH 2 to 12, and/or in a buffer containing another compound known or thought to contribute to altered stability e.g., surfactants, EDTA, EGTA, wheat flour components, or any other relevant additives. Filters so treated for a specified time are then rinsed briefly in deionized water and placed on plates for activity detection as described above. The conditions are chosen such that stabilized variants show increased enzymatic activity relative to the parent after incubation on the detection media.

To screen for variants with altered thermostability, filters with bound variants are incubated in buffer at a given pH (e.g., in the range from pH 2-12) at an elevated temperature (e.g., in the range from 50°-110°C) for a time period (e.g., from 1-20 minutes) to inactivate nearly all of the parent maltogenic alpha-amylase, rinsed in water, then placed directly on a detection plate containing immobilized Cibacron Red labelled amylopectin and incubated until activity is detectable. Similarly, pH dependent stability can be screened for by adjusting the pH of the buffer in the above inactivation step such that the parent maltogenic alpha-amylase is inactivated, thereby allowing detection of only those variants with increased stability at the pH in question. To screen

for variants with increased calcium-dependent stability calcium chelators, such as ethylene glycol-bis(β -aminoethyl ether) N,N,N',N'-tetraacetic acid (EGTA), is added to the inactivation buffer at a concentration such that the parent maltogenic alpha-amylase is inactivated under conditions further defined, such as buffer pH, temperature or a
5 specified length of incubation.

The variants of the invention may be suitably tested by assaying the starch-degrading activity of the variant, for instance by growing host cells transformed with a DNA sequence encoding a variant on a starch-containing agarose plate and identifying starch-degrading host cells as described above. Further testing in regard to altered
10 properties, including specific activity, substrate specificity, cleavage pattern, thermoactivation, thermostability, pH dependent activity or optimum, pH dependent stability, temperature dependent activity or optimum, transglycosylation activity, stability, and any other parameter of interest, may be performed on purified variants in accordance with methods known in the art as described below.

15 Degradation of β -limit dextrin by maltogenic alpha-amylase:

Another important parameter in the evaluation of the substrate specificity of maltogenic alpha-amylase variants may be the degree to which such enzymes are capable of degrading starch that has been exhaustively treated with the exoglycosylase β -amylase. To screen for variants which show patterns of degradation on such a
20 substrate differing from the patterns produced by the parent maltogenic alpha-amylase the following assay is performed: β -limit dextrin is prepared by incubating 25 ml 1% amylopectin in McIlvane buffer (48.5 mM citrate and 193 mM sodium phosphate pH 5.0) with 24 μ g/ml β -amylase overnight at 30°C. Unhydrolysed amylopectin (i.e., β -limit dextrin) is precipitated with 1 volume 98% ethanol, washed and redissolved in water. 1
25 ml β -limit dextrin is incubated with 18 μ l enzymes (at 2.2 mg/ml) and 100 μ l 0.2 M citrate-phosphate pH 5.0 for 2 hrs at 30°C and analysed by HPLC as described above. Total hydrolysis of β -limit dextrin is carried out in 2M HCl at 95°C. The concentration of reducing ends is measured by methods known in the art.

Calcium binding affinity

30 Unfolding of maltogenic alpha-amylases by exposure to heat or to denaturants such as guanidine hydrochloride is accompanied by a decrease in fluorescence, and loss of calcium ions leads to unfolding. Thus, the affinity of a maltogenic alpha-amylase variant for calcium can be measured by fluorescence measurements before and after incubation of the variant (e.g., at a concentration of 10 mg/ml) in a buffer (e.g., 50 mM
35 HEPES, pH 7) with different concentrations of calcium (e.g., in the range from

1 mM-100 mM) or of EGTA (e.g., in the range from 1-1000 mM) for a sufficiently long period of time (such as 22 hours at 55°C).

The measured fluorescence, F , is composed of contributions from the folded and unfolded forms of the enzyme. The following equation can be derived to describe the dependence of F on calcium concentration ($[Ca]$):

$$F = [Ca]/(K_{diss} + [Ca])(a_N - b_N \log([Ca])) + K_{diss}/(K_{diss} + [Ca])(a_U - b_U \log([Ca]))$$

where a_N is the fluorescence of the native (folded) form of the enzyme, b_N is the linear dependence of a_N on the logarithm of the calcium concentration (as observed experimentally), a_U is the fluorescence of the unfolded form and b_U is the linear dependence of a_U on the logarithm of the calcium concentration. K_{diss} is the apparent calcium binding constant for an equilibrium process as follows:

$$K_{diss}$$

$N-Ca \rightleftharpoons U + Ca$ (N = native enzyme; U = unfolded enzyme)

In fact, unfolding proceeds extremely slowly and is irreversible. The rate of unfolding is dependent on calcium concentration, and such dependency for a given enzyme provides a measure of the calcium binding affinity of the enzyme. By defining a standard set of reaction conditions (e.g., 22 hours at 55°C), a meaningful comparison of K_{diss} for different maltogenic alpha-amylase variants can be made.

Industrial Applications

The maltogenic alpha-amylase variants of the invention possesses valuable properties which may be advantageously used in various industrial applications. In particular, the enzyme finds potential application for retarding or preventing retrogradation, and thus the staling, of starch based food such as common in the baking industry.

The variant may be used for the preparation of bread and other bread products in accordance with conventional techniques known in the art.

It is believed that the modification of the starch fraction by use of the present invention results in increased volume in baked products and improved organoleptic qualities, such as flavour, mouth feel, palatability, aroma and crust colour.

The maltogenic alpha-amylase variant may be used as the only enzyme or as a major enzymatic activity in combination with one or more additional enzymes, such as xylanase, lipase, glucose oxidase and other oxidoreductases, or an amylolytic enzyme.

The enzyme variants of the invention also find industrial applicability as a component in washing, dishwashing and hard-surface cleaning detergent compositions. Some variants are particularly useful in a process for the manufacture of

linear oligosaccharides, or in the production of sweeteners and ethanol from starch, and/or for textile desizing. Conditions for conventional starch conversion processes, including starch liquefaction and/or saccharification processes, are described in, e.g., US 3,912,590 and in EP patent publications Nos. 252,730 and 63,909.

- 5 The invention is further illustrated with reference to the following examples which are not intended to be in any way limiting to the scope of the invention as claimed.

Determination of maltogenic amylase in MANU

- One Maltogenic Amylase Novo Unit (MANU) is the amount of enzyme which
10 under standard will cleave one μmol maltotriose per minute. The standard conditions are 10 mg/ml maltotriose, 37°C, pH 5.0, 30 minutes reaction time.

The pH dependence is found by repeating this measurement at the same conditions, but at different pH values.

EXAMPLES

- 15 **Example 1: Construction of a variant of Novamyl with altered pH dependent activity**

- Novamyl is expressed in *Bacillus subtilis* from a plasmid denoted herein as pLBei010. This plasmid contains *amyM* in which the expression of *amyM* is directed by its own promoter and the complete gene encoding Novamyl, e.g., as contained in the
20 strain DSM 11837. The plasmid contains the origin of replication, *ori*, from plasmid pUB110 and an kanamycin resistance marker for selection purposes. pLBei010 is shown in Fig. 1.

Primer sequences

- Site directed mutants of Novamyl were constructed by the megaprimer method
25 essentially as described by Kammann et al. (1989). Briefly, a mutagenic oligonucleotide primer is used together in a PCR reaction with a suitable opposite DNA strand end primer to create a preliminary PCR product. This product is then used as a megaprimer together with another opposite DNA strand end primer to create a double-stranded DNA product. The product of the final PCR reaction was routinely used to replace a
30 corresponding DNA fragment in the pLBei010 plasmid by standard cloning procedures. Mutants were transformed directly into *Bacillus subtilis* strain SHa273, a derivative of *Bacillus subtilis* 168 which is *apr*⁻, *npr*⁻, *amyE*⁻, *amyR2*⁻ and prepared by methods known in the art.

Oligonucleotide primers used in the construction of described variants are as listed below:

Variant Sequence (5' → 3')

F188H: SEQ ID NO: 3

5 F188E: SEQ ID NO: 4

F284E: SEQ ID NO: 5

F284D: SEQ ID NO: 6

F284K: SEQ ID NO: 7

N327D: SEQ ID NO: 8

10 Variant Sequence (3' → 5')

T288K: SEQ ID NO: 9

T288R: SEQ ID NO: 10

Aspartate variants of F284, T288 and N327 were obtained using primer A189 (SEQ ID NO: 11) and B649 (SEQ ID NO: 12) as end-primers.

15 F188-variants F188L, T189Y were obtained using primer A82 (SEQ ID NO: 13) and B346 (SEQ ID NO: 14) as end-primers.

PCR products with the desired modification(s) were purified, digested with appropriate enzymes, separated by agarose gel electrophoresis and extracted, ethanol precipitated in the presence of glycogen, resuspended in H₂O, ligated to pLBei010
20 which had been digested with the same appropriate enzymes, and transformed into *Bacillus subtilis* SHa273. Transformants were checked for size by colony PCR and for the insertion or removal of specific restriction sites by restriction enzyme digestion. Positive colonies were verified by DNA sequencing methods as described in the art.

Fermentation

25 The *B. subtilis* SHa273 mutant clones were grown overnight on LB-Kana (10 µg/ml)-Starch plates at 37°C. The colonies from the plate were resuspended in 10 ml Luria broth. One-sixth of each of the suspensions were inoculated into a 500 ml shake flasks containing 100 ml PS-1 media, a soy meal/sucrose-based media, kanamycin for a final concentration of 10 µg/ml and 100 µl 5M NaOH. The pH was adjusted to 7.5 with
30 NaOH before inoculation. The cultures were incubated for five days at 30°C with shaking at 270-300 rpm.

Enzyme Purification

Large particles from the media were removed by flocculation before affinity chromatography. Superfloc C521 (American Cyanmide Company) was used as the
35 cationic flocculant and Superfloc A130 (American Cyanmide Company) as the anionic flocculant.

The culture suspension was diluted 1:1 with deionized water and the pH was adjusted to approx. 7.5. A volume of 0.01 ml of 50%_w CaCl₂ per ml diluted culture was added during stirring. A volume of 0.015 ml of 20%_w Na-aluminate per ml diluted culture was titrated with 20% formic acid, while keeping the pH between 7 and 8. While stirring 0.025 ml 10%_v of C521 per ml diluted culture was added, followed by 0.05 ml 1%_v A130 per ml diluted culture, or until flocculation was observed. The solution was centrifuged at 4500 rpm for 30 minutes. Filtration was performed using a filter of pore size of 0.45 µm to exclude larger particles and any remaining bacteria. The filtered solution was stored at -20°C.

10 Immobilization of α-cyclodextrin to DSV-agarose

One hundred mg of α-cyclodextrin of molecular weight 972.86g/mol (Fluka 28705) was dissolved in 20 ml coupling buffer (0.5M Na₂CO₃, pH 11). Ten ml of DSV-agarose (Mini-Leak, Medium 10-20 mmol/l of divinyl sulfone activated agarose (Kem-En-Tec) was washed thoroughly with deionized water, then dried by suction and transferred to the α-cyclodextrin solution. After the mixture had stirred for 24 hr at ambient temperature, the gel was washed with deionized water, followed by 0.5M KHCO₃. The gel was transferred to the blocking buffer (20ml 0.5M KHCO₃ + 1ml mercaptoethanol), stirred for 2 hr at ambient temperature, then washed with deionized water.

20 Affinity chromatography

The variants were purified by affinity chromatography using the Pharmacia FPLC System. A 0.04 volume of 1M Na-acetate pH 5 was added to the filtrate obtained by flocculation to adjust pH and CaCl₂ was added to a final concentration of 10⁻¹⁰ M. The solution was filtered and degassed. A Pharmacia XK16 column was prepared with ten ml of the immobilised α-cyclodextrin, then equilibrated in the equilibration buffer (25 mM Na-acetate pH 5) by washing with approximately 10 times the column volume. The filtrate was applied to the XK16 column, which was then washed with the equilibration buffer until protein could no longer be detected in the washing buffer. The column was washed with the equilibration buffer containing 0.5M NaCl to elute nonspecific material, followed by another wash with 2-3 times the column volume of the equilibration buffer. All washings were performed using a flow rate of 10ml/min. Specifically bound material was eluted using a solution of 2% α-cyclodextrin in the wash buffer and collected using the Pharmacia Liquid Chromatography Collector LCC-500 Plus using a flow rate of 5 ml/min.

Example 2: pH dependent activity of variants

The variants prepared in the preceding Example were tested for activity at various pH values as follows.

A colorimetric glucose oxidase-peroxidase assay for liberated glucose from maltotriose or amylopectin was used to determine the pH activity profiles of the enzyme variants (Glucose/GOD-Perid[®] Method, Boehringer Mannheim, Indianapolis IN). Activity was assayed in a buffer of 25 mM citrate-phosphate, 0.1mM CaCl₂ at pH values of 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8 and 8.6. The buffer pH was adjusted using NaOH and enzymes were diluted in 25 mM citrate-phosphate buffer pH 5. Measurements were taken in duplicate to obtain an average value. All values are relative to the pH at which the highest level of activity is seen.

The results, shown in the table below, indicate that each of the variants has an alteration in the pH dependent activity profile when compared to the parent Novamyl[®]. The highest level of activity for each variant is designated 100% and the activity of that variant measured at the other indicated pH values is a relative percentage of that maximum.

| Modifications | pH | | | | | | | | | | | | | |
|---------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| | 2.0 | 2.5 | 3.0 | 3.5 | 4.0 | 4.5 | 5.0 | 5.5 | 6.0 | 6.5 | 7.0 | 7.5 | 8.0 | 8.6 |
| None (parent) | 0 | 0 | 0 | 8 | 47 | 80 | 100 | 95 | 91 | 80 | 66 | 39 | 35 | 30 |
| F188H | 1 | 0 | 0 | 1 | 3 | 29 | 77 | 99 | 100 | 88 | 59 | 39 | 31 | 27 |
| F188E | 0 | 0 | 0 | 2 | 27 | 62 | 89 | 100 | 93 | 71 | 46 | 28 | 20 | 18 |
| T288R | 0 | 0 | 0 | 8 | 51 | 77 | 94 | 100 | 86 | 73 | 50 | 34 | 27 | 12 |
| N327D | 1 | 1 | 7 | 27 | 67 | 95 | 100 | 98 | 77 | 33 | 19 | 11 | 5 | 0 |

Further, a number of Novamyl variants were tested for activity at pH 4.0 and 5.0, taking the activity of Novamyl at the same pH as 100 %. The activity was determined by hydrolysis of maltotriose (10 mg/ml) at 60°C, 50 mM sodium acetate, 1 mM CaCl₂. The results are expressed as the ratio between activity at pH 5.0 and pH 4.0:

| Modifications | pH 5.0/pH 4.0 |
|---------------|---------------|
| N131D | 0.24 |
| I174Q | 0.31 |

| | |
|----------------------|------|
| G397P | 0.40 |
| H103Y | 0.40 |
| Δ 262-266 | 0.47 |
| S32Q | 0.53 |
| S32D | 0.55 |
| T142A+ D261G | 0.62 |
| G370N+ N371G | 0.66 |
| S32N | 0.68 |
| N176S | 0.79 |
| D17E | 0.80 |
| None (parent) | 1 |
| Δ 191 | 1.39 |
| 192-A-193 | 1.61 |
| I174E | 1.80 |
| 192-A-G-193 | 1.90 |
| Δ 192 | 2.22 |

The results demonstrate that variants with a higher or lower pH optimum can be obtained according to the invention.

Example 3: Thermostability of variants

5 Incubation at 80°C

The thermostability of a number of Novamyl variants was tested by incubating an aqueous solution at 80°C and pH 4.3 and measuring the residual amylase activity at various times. The parent enzyme, Novamyl, was included for comparison. The results are expressed as residual activity at various times in percent of initial activity:

10

| Modifications | 0 | 5 min. | 10 min. | 15 min. | 20 min. | 25 min. |
|----------------------------|----------|---------------|----------------|----------------|----------------|----------------|
| None (parent) | 100 | 23 | 9 | 3 | 1 | 0 |
| F188L+ V336L+ T525A | 100 | 63 | 49 | 48 | 52 | 47 |
| F188I+ Y422F+ I660V | 100 | 71 | 60 | 51 | 43 | 38 |
| N115D+ F188L | 100 | 73 | 60 | 51 | 44 | 39 |

| | | | | | | |
|--|-----|----|----|----|----|----|
| A30D+ K40R+ D261G | 100 | 38 | 24 | 15 | 13 | 10 |
| T142A+ N327S+ K425E+ K520R+ N595I | 100 | 47 | 39 | 25 | 19 | 11 |
| F188L+ D261G+ T288P | 100 | 60 | 67 | 66 | 63 | 67 |
| K40R+ F188L+ D261G+ A483T | 100 | 56 | 48 | 40 | 36 | 30 |
| T288K | 100 | 64 | 31 | 18 | 7 | 4 |

The above data show a clearly improved thermostability for the variants compared to the parent amylase.

Incubation at 85°C with calcium

- 5 The Novamyl variant S32E was tested by incubation with 1 mM Ca⁺⁺ at 85°C for 15 minutes. The variant showed a residual activity of 48 % whereas the parent enzyme (Novamyl) showed 32 % residual activity at the same conditions.

DSC

- 10 Further, the thermostability was tested for some Novamyl variants by DSC (differential scanning calorimetry) at pH 4.3 or 5.5. Again, the parent amylase was included for comparison. The results are expressed as the denaturation temperature (T_m):

| Modifications | T_m at pH 4.3 | T_m at pH 5.5 |
|--|--------------------------------|--------------------------------|
| None (parent) | 79°C | 88°C |
| N115D+ F188L | 86°C | 92°C |
| T142A+ N327S+ K425E+ K520R+ N595I | not determined | 93°C |

- 15 The results show improved thermostability for both variants.

Example 4: Specific activity of variants

Amylase activity was determined by a colorimetric measurement after action on Phadebas tablets at pH 5.0 and 60°C. The results for two Novamyl variants, relative to Novamyl were as follows:

| Modifications | Relative amylase activity |
|--------------------|---------------------------|
| None (parent) | 100 |
| 192-A-193 | 110 |
| Δ (191-195) | 300 |

The specific activity was further tested by action on maltotriose at pH 4.0, 60°C by the MANU method described above. The results showed that the variant G370N, N371G has a maltotriose activity of 106 % compared to Novamyl.

5 Example 5: Inhibition of retrogradation

The efficiency of Novamyl and Novamyl variants to inhibit retrogradation was determined as follows:

730 mg of 50 % (w/w) amylopectin slurry in 0.1 M sodium acetate, at a selected pH (3.7, 4.3 or 5.5) was mixed with 20 μ l of an enzyme sample, and the mixture was incubated in a sealed ampoule for 1 hour at 40°C, followed by incubation at 100 °C for 1 hour in order to gelatinize the samples. The sample was then aged for 7 days at room temperature to allow recrystallization of the amylopectin. A control without enzyme was included.

After aging, DSC was performed on the sample by scanning from 5°C to 95°C at a constant scan rate of 90°C/hour. The area under the first endothermic peak in the thermogram was taken to represent the amount of retrograded amylopectin, and the relative inhibition of retrogradation was taken as the area reduction (in %) relative to the control without enzyme.

In the table below, the efficiency of the enzyme is expressed as the ratio of the relative inhibition of retrogradation to the enzyme dosage (in MANU/ml):

| pH | Modifications | MANU/ml | Relative inhibition | Efficiency |
|-----|-----------------------------------|---------|---------------------|------------|
| 3.7 | A30D+ K40R+ D261G | 0.23 | 0.38 | 1.7 |
| 3.7 | T142A+ N327S+ K425E+ K520R+ N595I | 0.07 | 0.29 | 4.1 |
| 3.7 | None (parent) | 0.27 | 0.38 | 1.4 |
| 4.3 | N115D+ F188L | 0.01 | 0.18 | 18 |
| 4.3 | None (parent) | 0.27 | 0.43 | 1.6 |

| | | | | |
|-----|----------------------------------|------|------|-----|
| 5.5 | Δ (191-195)+ F188L+ T189Y | 0.02 | 0.12 | 6 |
| 5.5 | Δ (191-195) | 0.02 | 0.14 | 7 |
| 5.5 | Δ (191-195) | 0.05 | 0.31 | 6.2 |
| 5.5 | N115D+ F188L | 0.01 | 0.39 | 39 |
| 5.5 | T142A+ D261G | 0.14 | 0.53 | 3.8 |
| 5.5 | None (parent) | 0.27 | 0.49 | 1.8 |

The results demonstrate that a number of variants are more efficient than the parent amylase to inhibit retrogradation.

Example 6: Anti-staling effect of variants

5 Bread was made by the European Straight Dough method or from sour dough with or without addition of enzymes, and loaves were baked in lidded pans, to avoid volume effects. The bread was allowed to cool for 2 hours, and the texture was analyzed. The remaining loaves were then wrapped in plastic bags and stored at room temperature for texture analysis after 1, 4 and 7 days.

10 The texture analysis of each loaf was done by cutting 4 slices; the force was measured at 25 % compression (P1), at 40% compression (P2) and after keeping 40% compression constant for 30 sec. (P3). P1 was taken as the firmness, and the ratio (P3/P2) was taken as the elasticity of the crumb. The extent of retrogradation after 7 days storage was determined by DSC as described in Example 7.

15 European Straight Dough (pH5.5-6.0)

A Novamyl variant (T142A+ N327S+ K425E+ K520R+ N595I) was tested at dosages in the range of 0-2 mg enzyme/kg flour, and the parent enzyme (Novamyl) was used for comparison.

20 The results showed that at equal dosages, the variant gives better elasticity (P3/P2) than the parent enzyme after two hours and 1 day. The results after 7 days showed that the variant at dosages of 1-2 mg/kg gave significantly softer crumb (lower firmness, P1) than the parent enzyme at the same dosage. Thus, the variant has a better anti-staling effect throughout a 7-day storage period.

Sour dough (pH approx. 4.5)

25 A Novamyl variant (F188L+ D261G+ T288P) was tested in sour dough, and the parent enzyme (Novamyl) was used for comparison. The following results were

obtained for firmness (P1) after 7 days, elasticity (P3/P2) after 4 and 7 days and retrogradation after 7 days:

| Enzyme | Dosage mg/kg flour | Firmness (P1) after 7 days |
|---------|-----------------------|-------------------------------|
| None | 0 | 2590 |
| Parent | 1 | 2031 |
| | 3 | 1912 |
| | 13 | 1570 |
| Variant | 1 | 1436 |
| | 3 | 1226 |

| Enzyme | Dosage mg/kg flour | Elasticity 4 days | Elasticity 7 days |
|---------|-----------------------|----------------------|----------------------|
| None | 0 | 0.49 | 0.47 |
| Parent | 1 | 0.51 | 0.52 |
| | 3 | 0.53 | 0.51 |
| | 13 | 0.53 | 0.51 |
| Variant | 1 | 0.59 | 0.57 |
| | 3 | 0.57 | 0.58 |

| Enzyme | Dosage mg/kg flour | Retrogradation, 7 days (relative to control) |
|---------|-----------------------|---|
| None | 0 | 100 % |
| Parent | 1 | 100 % |
| | 3 | 63 % |
| | 13 | 32 % |
| Variant | 1 | 46 % |
| | 3 | 20 % |

The results show that the variant has a markedly improved effect on texture evaluated as firmness and elasticity in sour dough at pH 4.5. A dosage of 1-3 mg/kg of the variant is superior to 13 mg/kg of the parent enzyme on all parameters tested, and the elasticity achieved with the variant cannot be matched by the parent enzyme at any dosage.

Example 7: Cleavage pattern of variants

The cleavage pattern in starch hydrolysis was compared for two variants and the parent enzyme, Novamyl.

The results below indicate % by weight of each oligosaccharide (G1-G8) formed after 24 hours incubation in 1% (w/v) starch using 50 mM sodium acetate, 1 mM CaCl₂, pH 5.0 at 50 °C. The oligosaccharides were identified and quantitated using HPLC.

| Oligosaccharide | Parent | Δ (191-195) | N115D+ F188L |
|-----------------|--------|--------------------|--------------|
| G8 | - | 1.7 | - |
| G7 | - | 2.6 | - |
| G6 | - | 7.5 | 1.4 |
| G5 | - | 10.1 | 2.1 |
| G4 | - | 21.1 | 11.3 |
| G3 | - | 28.7 | 10.7 |
| G2 | 96.5 | 28.3 | 61.9 |
| G1 | 3.5 | - | 12.6 |

The results demonstrate a significantly altered cleavage pattern. Novamyl after 24 hours produces mainly maltose and virtually no higher oligosaccharides. In contrast, the two variants produce significant amounts of maltotriose and higher oligosaccharides.

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| | | | | | | | | | | | | | | | | | | | |
|----|-----|-------|---|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 1 | N | SER A | 1 | 10.254 | 56.595 | 38.175 | 1.00 | 15.64 | 7 | 43 | CD | LYS A | 7 | 18.160 | 63.123 | 46.350 | 1.00 | 9.80 | 6 |
| 2 | CA | SER A | 1 | 11.216 | 55.462 | 37.898 | 1.00 | 15.87 | 6 | 44 | CE | LYS A | 7 | 17.698 | 64.488 | 45.795 | 1.00 | 10.87 | 6 |
| 3 | C | SER A | 1 | 12.466 | 55.723 | 38.726 | 1.00 | 14.53 | 6 | 45 | NZ | LYS A | 7 | 17.114 | 64.187 | 44.425 | 1.00 | 11.38 | 7 |
| 4 | O | SER A | 1 | 12.585 | 56.773 | 39.369 | 1.00 | 15.99 | 8 | 46 | N | GLY A | 8 | 21.036 | 58.214 | 45.577 | 1.00 | 13.10 | 7 |
| 5 | CB | SER A | 1 | 11.527 | 55.345 | 36.397 | 1.00 | 21.54 | 6 | 47 | CA | GLY A | 8 | 21.604 | 56.982 | 46.166 | 1.00 | 12.31 | 6 |
| 6 | OG | SER A | 1 | 12.305 | 56.503 | 36.045 | 1.00 | 20.33 | 8 | 48 | C | GLY A | 8 | 22.718 | 56.358 | 45.340 | 1.00 | 14.02 | 6 |
| 7 | N | SER A | 2 | 13.466 | 54.795 | 38.551 | 1.00 | 18.07 | 7 | 49 | O | GLY A | 8 | 23.109 | 55.205 | 45.579 | 1.00 | 13.36 | 8 |
| 8 | CA | SER A | 2 | 14.705 | 55.061 | 39.291 | 1.00 | 19.33 | 6 | 50 | N | ASP A | 9 | 23.133 | 57.048 | 44.293 | 1.00 | 11.90 | 7 |
| 9 | C | SER A | 2 | 15.621 | 56.069 | 38.559 | 1.00 | 15.87 | 6 | 51 | CA | ASP A | 9 | 24.049 | 56.447 | 43.319 | 1.00 | 11.74 | 6 |
| 10 | O | SER A | 2 | 16.573 | 56.563 | 39.209 | 1.00 | 16.73 | 8 | 52 | C | ASP A | 9 | 25.478 | 56.996 | 43.442 | 1.00 | 10.18 | 6 |
| 11 | CB | SER A | 2 | 15.490 | 53.735 | 39.422 | 1.00 | 26.53 | 6 | 106 | CB | ILE A | 15 | 37.192 | 59.653 | 28.343 | 1.00 | 10.73 | 6 |
| 12 | OG | SER A | 2 | 15.918 | 53.392 | 38.123 | 1.00 | 21.07 | 8 | 107 | CG1 | ILE A | 15 | 37.106 | 60.975 | 29.131 | 1.00 | 11.86 | 6 |
| 13 | N | SER A | 3 | 15.136 | 56.545 | 37.384 | 1.00 | 12.71 | 7 | 108 | CG2 | ILE A | 15 | 37.626 | 60.014 | 26.904 | 1.00 | 12.56 | 6 |
| 14 | CA | SER A | 3 | 15.956 | 57.522 | 36.680 | 1.00 | 13.38 | 6 | 109 | CD1 | ILE A | 15 | 36.181 | 62.091 | 28.574 | 1.00 | 15.42 | 6 |
| 15 | C | SER A | 3 | 15.873 | 58.916 | 37.316 | 1.00 | 12.57 | 6 | 110 | N | ILE A | 16 | 34.926 | 57.450 | 26.561 | 1.00 | 10.37 | 7 |
| 16 | O | SER A | 3 | 16.759 | 59.749 | 37.029 | 1.00 | 15.22 | 8 | 111 | CA | ILE A | 16 | 34.728 | 56.178 | 25.868 | 1.00 | 11.03 | 6 |
| 17 | CB | SER A | 3 | 15.434 | 57.682 | 35.219 | 1.00 | 16.30 | 6 | 112 | C | ILE A | 16 | 35.990 | 55.729 | 25.099 | 1.00 | 12.23 | 6 |
| 18 | OG | SER A | 3 | 15.593 | 56.381 | 34.568 | 1.00 | 23.61 | 8 | 113 | O | ILE A | 16 | 36.342 | 54.511 | 25.184 | 1.00 | 11.07 | 8 |
| 19 | N | ALA A | 4 | 14.811 | 59.222 | 38.050 | 1.00 | 10.88 | 7 | 114 | CB | ILE A | 16 | 33.578 | 56.292 | 24.863 | 1.00 | 10.56 | 6 |
| 20 | CA | ALA A | 4 | 14.574 | 60.623 | 38.384 | 1.00 | 11.38 | 6 | 115 | CG1 | ILE A | 16 | 32.240 | 56.387 | 25.709 | 1.00 | 11.92 | 6 |
| 21 | C | ALA A | 4 | 15.599 | 61.115 | 39.409 | 1.00 | 12.81 | 6 | 116 | CG2 | ILE A | 16 | 33.444 | 55.053 | 23.953 | 1.00 | 11.18 | 6 |
| 22 | O | ALA A | 4 | 15.888 | 62.314 | 39.355 | 1.00 | 12.58 | 8 | 117 | CD1 | ILE A | 16 | 31.115 | 56.958 | 24.823 | 1.00 | 13.67 | 6 |
| 23 | CB | ALA A | 4 | 13.132 | 60.682 | 38.956 | 1.00 | 14.28 | 6 | 118 | N | ASP A | 17 | 36.565 | 56.624 | 24.314 | 1.00 | 10.08 | 7 |
| 24 | N | SER A | 5 | 15.968 | 60.306 | 40.380 | 1.00 | 13.21 | 7 | 119 | CA | ASP A | 17 | 37.730 | 56.165 | 23.518 | 1.00 | 8.61 | 6 |
| 25 | CA | SER A | 5 | 16.905 | 60.780 | 41.427 | 1.00 | 14.29 | 6 | 120 | C | ASP A | 17 | 38.911 | 55.693 | 24.346 | 1.00 | 10.86 | 6 |
| 26 | C | SER A | 5 | 18.163 | 59.941 | 41.357 | 1.00 | 16.01 | 6 | 121 | O | ASP A | 17 | 39.777 | 54.987 | 23.831 | 1.00 | 11.03 | 8 |
| 27 | O | SER A | 5 | 18.053 | 58.724 | 41.237 | 1.00 | 16.41 | 8 | 122 | CB | ASP A | 17 | 38.184 | 57.422 | 22.675 | 1.00 | 11.30 | 6 |
| 28 | CB | SER A | 5 | 16.218 | 60.613 | 42.785 | 1.00 | 15.57 | 6 | 123 | CG | ASP A | 17 | 39.380 | 57.017 | 21.755 | 1.00 | 9.77 | 6 |
| 29 | OG | SER A | 5 | 17.193 | 60.855 | 43.843 | 1.00 | 13.17 | 8 | 124 | OD1 | ASP A | 17 | 39.105 | 56.206 | 20.852 | 1.00 | 11.65 | 8 |
| 30 | N | VAL A | 6 | 19.340 | 60.530 | 41.476 | 1.00 | 10.07 | 7 | 125 | OD2 | ASP A | 17 | 40.480 | 57.562 | 21.970 | 1.00 | 11.48 | 8 |
| 31 | CA | VAL A | 6 | 20.589 | 59.751 | 41.567 | 1.00 | 10.13 | 6 | 126 | N | ARG A | 18 | 38.972 | 55.999 | 25.646 | 1.00 | 9.54 | 7 |
| 32 | C | VAL A | 6 | 21.169 | 59.955 | 42.963 | 1.00 | 10.99 | 6 | 127 | CA | ARG A | 18 | 40.113 | 55.719 | 26.527 | 1.00 | 8.38 | 6 |
| 33 | O | VAL A | 6 | 22.349 | 59.685 | 43.172 | 1.00 | 10.81 | 8 | 128 | C | ARG A | 18 | 39.826 | 54.720 | 27.608 | 1.00 | 9.97 | 6 |
| 34 | CB | VAL A | 6 | 21.639 | 60.160 | 40.513 | 1.00 | 13.85 | 6 | 129 | O | ARG A | 18 | 40.643 | 54.490 | 28.501 | 1.00 | 13.32 | 8 |
| 35 | CG1 | VAL A | 6 | 21.002 | 59.694 | 39.148 | 1.00 | 15.29 | 6 | 130 | CB | ARG A | 18 | 40.537 | 57.083 | 27.137 | 1.00 | 11.02 | 6 |
| 36 | CG2 | VAL A | 6 | 21.874 | 61.656 | 40.459 | 1.00 | 12.12 | 6 | 131 | CG | ARG A | 18 | 40.931 | 58.139 | 26.063 | 1.00 | 9.63 | 6 |
| 37 | N | LYS A | 7 | 20.369 | 60.349 | 43.964 | 1.00 | 10.30 | 7 | 132 | CD | ARG A | 18 | 42.135 | 57.721 | 25.237 | 1.00 | 9.86 | 6 |
| 38 | CA | LYS A | 7 | 20.901 | 60.604 | 45.331 | 1.00 | 9.78 | 6 | 133 | NE | ARG A | 18 | 42.280 | 58.523 | 23.969 | 1.00 | 10.16 | 7 |
| 39 | C | LYS A | 7 | 21.508 | 59.360 | 46.015 | 1.00 | 12.06 | 6 | 134 | CZ | ARG A | 18 | 43.103 | 59.578 | 23.903 | 1.00 | 13.46 | 6 |
| 40 | O | LYS A | 7 | 22.382 | 59.560 | 46.857 | 1.00 | 12.59 | 8 | 135 | NH1 | ARG A | 18 | 43.748 | 60.063 | 24.966 | 1.00 | 12.03 | 7 |
| 41 | CB | LYS A | 7 | 19.830 | 61.187 | 46.264 | 1.00 | 11.40 | 6 | 136 | NH2 | ARG A | 18 | 43.350 | 60.181 | 22.725 | 1.00 | 10.43 | 7 |
| 42 | CG | LYS A | 7 | 19.414 | 62.588 | 45.680 | 1.00 | 12.09 | 6 | 137 | N | PHE A | 19 | 38.648 | 54.007 | 27.497 | 1.00 | 11.25 | 7 |

| | | | | | | | | | | | | | | | | | | | |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 138 | CA | PHE A | 19 | 38.296 | 53.057 | 28.601 | 1.00 | 10.13 | 6 | 180 | N | THR A | 24 | 37.681 | 45.659 | 18.083 | 1.00 | 15.02 | 7 |
| 139 | C | PHE A | 19 | 38.543 | 51.614 | 28.192 | 1.00 | 12.61 | 6 | 181 | CA | THR A | 24 | 38.769 | 46.308 | 17.340 | 1.00 | 16.37 | 6 |
| 140 | O | PHE A | 19 | 39.528 | 51.024 | 28.677 | 1.00 | 12.51 | 8 | 182 | C | THR A | 24 | 38.381 | 46.606 | 15.923 | 1.00 | 15.39 | 6 |
| 141 | CB | PHE A | 19 | 36.798 | 53.294 | 28.945 | 1.00 | 13.20 | 6 | 183 | O | THR A | 24 | 39.124 | 47.376 | 15.252 | 1.00 | 16.40 | 8 |
| 142 | CG | PHE A | 19 | 36.342 | 52.543 | 30.189 | 1.00 | 12.09 | 6 | 184 | CB | THR A | 24 | 40.033 | 45.402 | 17.367 | 1.00 | 18.68 | 6 |
| 143 | CD1 | PHE A | 19 | 36.849 | 52.908 | 31.423 | 1.00 | 12.96 | 6 | 185 | OG1 | THR A | 24 | 39.710 | 44.147 | 16.673 | 1.00 | 17.99 | 8 |
| 144 | CD2 | PHE A | 19 | 35.472 | 51.447 | 30.058 | 1.00 | 13.30 | 6 | 186 | CG2 | THR A | 24 | 40.478 | 45.112 | 18.772 | 1.00 | 22.45 | 6 |
| 145 | CE1 | PHE A | 19 | 36.500 | 52.187 | 32.563 | 1.00 | 16.46 | 6 | 187 | N | THR A | 25 | 37.228 | 46.150 | 15.423 | 1.00 | 16.09 | 7 |
| 146 | CE2 | PHE A | 19 | 35.184 | 50.719 | 31.215 | 1.00 | 12.02 | 6 | 188 | CA | THR A | 25 | 36.864 | 46.330 | 14.019 | 1.00 | 16.07 | 6 |
| 147 | CZ | PHE A | 19 | 35.638 | 51.089 | 32.482 | 1.00 | 11.98 | 6 | 189 | C | THR A | 25 | 36.349 | 47.743 | 13.724 | 1.00 | 16.52 | 6 |
| 148 | N | TYR A | 20 | 37.844 | 51.054 | 27.199 | 1.00 | 11.48 | 7 | 190 | O | THR A | 25 | 36.215 | 48.013 | 12.538 | 1.00 | 20.25 | 8 |
| 149 | CA | TYR A | 20 | 38.154 | 49.694 | 26.772 | 1.00 | 11.40 | 6 | 191 | CB | THR A | 25 | 35.780 | 45.366 | 13.475 | 1.00 | 20.06 | 6 |
| 150 | C | TYR A | 20 | 37.730 | 49.476 | 25.321 | 1.00 | 10.89 | 6 | 192 | OG1 | THR A | 25 | 34.475 | 45.532 | 14.010 | 1.00 | 18.04 | 8 |
| 151 | O | TYR A | 20 | 36.593 | 49.813 | 24.934 | 1.00 | 11.80 | 8 | 193 | CG2 | THR A | 25 | 36.248 | 43.924 | 13.739 | 1.00 | 21.26 | 6 |
| 152 | CB | TYR A | 20 | 37.417 | 48.696 | 27.719 | 1.00 | 12.88 | 6 | 194 | N | ASN A | 26 | 36.066 | 48.509 | 14.802 | 1.00 | 13.98 | 7 |
| 153 | CG | TYR A | 20 | 37.927 | 47.270 | 27.504 | 1.00 | 13.88 | 6 | 195 | CA | ASN A | 26 | 35.577 | 49.871 | 14.471 | 1.00 | 12.49 | 6 |
| 154 | CD1 | TYR A | 20 | 39.216 | 46.968 | 27.943 | 1.00 | 14.05 | 6 | 196 | C | ASN A | 26 | 36.689 | 50.862 | 14.772 | 1.00 | 13.05 | 6 |
| 155 | CD2 | TYR A | 20 | 37.160 | 46.285 | 26.932 | 1.00 | 15.80 | 6 | 197 | O | ASN A | 26 | 36.435 | 52.053 | 14.825 | 1.00 | 11.58 | 8 |
| 156 | CE1 | TYR A | 20 | 39.717 | 45.678 | 27.800 | 1.00 | 16.74 | 6 | 198 | CB | ASN A | 26 | 34.283 | 50.103 | 15.246 | 1.00 | 13.85 | 6 |
| 157 | CE2 | TYR A | 20 | 37.658 | 44.982 | 26.795 | 1.00 | 19.32 | 6 | 199 | CG | ASN A | 26 | 34.435 | 49.981 | 16.739 | 1.00 | 15.62 | 6 |
| 158 | CZ | TYR A | 20 | 38.935 | 44.710 | 27.214 | 1.00 | 19.70 | 6 | 200 | OD1 | ASN A | 26 | 35.558 | 50.066 | 17.224 | 1.00 | 12.89 | 8 |
| 159 | OH | TYR A | 20 | 39.458 | 43.422 | 27.062 | 1.00 | 22.69 | 8 | 201 | ND2 | ASN A | 26 | 33.339 | 49.796 | 17.497 | 1.00 | 16.36 | 7 |
| 160 | N | ASP A | 21 | 38.662 | 48.893 | 24.586 | 1.00 | 13.46 | 7 | 202 | N | ASN A | 27 | 37.946 | 50.401 | 14.890 | 1.00 | 14.79 | 7 |
| 161 | CA | ASP A | 21 | 38.414 | 48.628 | 23.134 | 1.00 | 14.35 | 6 | 203 | CA | ASN A | 27 | 38.972 | 51.353 | 15.290 | 1.00 | 12.19 | 6 |
| 162 | C | ASP A | 21 | 37.754 | 47.226 | 23.097 | 1.00 | 14.61 | 6 | 204 | C | ASN A | 27 | 39.404 | 52.337 | 14.189 | 1.00 | 13.62 | 6 |
| 163 | O | ASP A | 21 | 38.426 | 46.196 | 23.063 | 1.00 | 13.84 | 8 | 205 | O | ASN A | 27 | 39.775 | 53.461 | 14.499 | 1.00 | 14.13 | 8 |
| 164 | CB | ASP A | 21 | 39.746 | 48.665 | 22.413 | 1.00 | 14.54 | 6 | 206 | CB | ASN A | 27 | 40.235 | 50.575 | 15.662 | 1.00 | 12.10 | 6 |
| 165 | CG | ASP A | 21 | 39.678 | 48.444 | 20.909 | 1.00 | 17.30 | 6 | 207 | CG | ASN A | 27 | 40.150 | 49.884 | 17.001 | 1.00 | 15.80 | 6 |
| 166 | OD1 | ASP A | 21 | 38.565 | 48.288 | 20.425 | 1.00 | 12.67 | 8 | 208 | OD1 | ASN A | 27 | 39.065 | 49.932 | 17.554 | 1.00 | 12.92 | 8 |
| 167 | OD2 | ASP A | 21 | 40.759 | 48.450 | 20.282 | 1.00 | 15.87 | 8 | 209 | ND2 | ASN A | 27 | 41.187 | 49.291 | 17.571 | 1.00 | 15.14 | 7 |
| 168 | N | GLY A | 22 | 36.430 | 47.219 | 23.040 | 1.00 | 12.11 | 7 | 210 | N | ASN A | 28 | 39.211 | 51.954 | 12.920 | 1.00 | 14.26 | 7 |
| 169 | CA | GLY A | 22 | 35.683 | 45.934 | 23.110 | 1.00 | 15.21 | 6 | 211 | CA | ASN A | 28 | 39.604 | 52.918 | 11.854 | 1.00 | 15.71 | 6 |
| 170 | C | GLY A | 22 | 35.482 | 45.410 | 21.664 | 1.00 | 18.33 | 6 | 212 | C | ASN A | 28 | 38.672 | 52.705 | 10.661 | 1.00 | 14.39 | 6 |
| 171 | O | GLY A | 22 | 35.034 | 44.264 | 21.516 | 1.00 | 17.21 | 8 | 213 | O | ASN A | 28 | 39.059 | 52.148 | 9.622 | 1.00 | 16.82 | 8 |
| 172 | N | ASP A | 23 | 35.786 | 46.189 | 20.639 | 1.00 | 13.30 | 7 | 214 | CB | ASN A | 28 | 41.036 | 52.497 | 11.478 | 1.00 | 13.79 | 6 |
| 173 | CA | ASP A | 23 | 35.505 | 45.770 | 19.261 | 1.00 | 14.68 | 6 | 215 | CG | ASN A | 28 | 41.790 | 53.538 | 10.656 | 1.00 | 21.29 | 6 |
| 174 | C | ASP A | 23 | 36.634 | 46.389 | 18.425 | 1.00 | 14.54 | 6 | 216 | OD1 | ASN A | 28 | 41.391 | 54.685 | 10.535 | 1.00 | 17.46 | 8 |
| 175 | O | ASP A | 23 | 36.570 | 47.597 | 18.138 | 1.00 | 13.39 | 8 | 217 | ND2 | ASN A | 28 | 42.936 | 53.086 | 10.108 | 1.00 | 24.72 | 7 |
| 176 | CB | ASP A | 23 | 34.163 | 46.271 | 18.762 | 1.00 | 13.59 | 6 | 218 | N | PRO A | 29 | 37.442 | 53.154 | 10.790 | 1.00 | 15.04 | 7 |
| 177 | CG | ASP A | 23 | 33.889 | 45.785 | 17.319 | 1.00 | 16.74 | 6 | 219 | CA | PRO A | 29 | 36.430 | 52.993 | 9.742 | 1.00 | 17.37 | 6 |
| 178 | OD1 | ASP A | 23 | 34.805 | 45.200 | 16.750 | 1.00 | 17.96 | 8 | 220 | C | PRO A | 29 | 36.734 | 53.802 | 8.507 | 1.00 | 18.08 | 6 |
| 179 | OD2 | ASP A | 23 | 32.782 | 46.058 | 16.872 | 1.00 | 16.43 | 8 | 221 | O | PRO A | 29 | 37.259 | 54.906 | 8.580 | 1.00 | 16.51 | 8 |

| | | | | | | | | | | | | | | | | | | | |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 222 | CB | PRO A | 29 | 35.087 | 53.483 | 10.312 | 1.00 | 17.71 | 6 | 264 | O | LEU A | 35 | 42.472 | 58.755 | 15.182 | 1.00 | 14.18 | 8 |
| 223 | CG | PRO A | 29 | 35.394 | 53.615 | 11.787 | 1.00 | 17.95 | 6 | 265 | CB | LEU A | 35 | 40.784 | 59.737 | 13.090 | 1.00 | 10.53 | 6 |
| 224 | CD | PRO A | 29 | 36.907 | 53.841 | 11.957 | 1.00 | 15.54 | 6 | 266 | CG | LEU A | 35 | 40.170 | 60.460 | 11.891 | 1.00 | 12.89 | 6 |
| 225 | N | ALA A | 30 | 36.329 | 53.244 | 7.331 | 1.00 | 16.99 | 7 | 267 | CD1 | LEU A | 35 | 38.783 | 61.033 | 12.240 | 1.00 | 13.47 | 6 |
| 226 | CA | ALA A | 30 | 36.533 | 54.024 | 6.117 | 1.00 | 19.06 | 6 | 268 | CD2 | LEU A | 35 | 41.090 | 61.613 | 11.433 | 1.00 | 15.36 | 6 |
| 227 | C | ALA A | 30 | 35.841 | 55.375 | 6.161 | 1.00 | 16.15 | 6 | 269 | N | TYR A | 36 | 43.025 | 57.036 | 13.757 | 1.00 | 13.30 | 7 |
| 228 | O | ALA A | 30 | 36.398 | 56.355 | 5.599 | 1.00 | 18.27 | 8 | 270 | CA | TYR A | 36 | 43.335 | 56.061 | 14.796 | 1.00 | 13.00 | 6 |
| 229 | CB | ALA A | 30 | 35.998 | 53.268 | 4.880 | 1.00 | 21.27 | 6 | 271 | C | TYR A | 36 | 44.826 | 55.913 | 15.032 | 1.00 | 15.18 | 6 |
| 230 | N | LYS A | 31 | 34.697 | 55.514 | 6.833 | 1.00 | 15.01 | 7 | 272 | O | TYR A | 36 | 45.610 | 55.855 | 14.049 | 1.00 | 15.86 | 8 |
| 231 | CA | LYS A | 31 | 34.012 | 56.812 | 6.886 | 1.00 | 14.64 | 6 | 273 | CB | TYR A | 36 | 42.749 | 54.728 | 14.291 | 1.00 | 13.61 | 6 |
| 232 | C | LYS A | 31 | 34.944 | 57.908 | 7.416 | 1.00 | 15.07 | 6 | 274 | CG | TYR A | 36 | 43.149 | 53.492 | 15.076 | 1.00 | 12.30 | 6 |
| 233 | O | LYS A | 31 | 34.722 | 59.094 | 7.172 | 1.00 | 14.25 | 8 | 275 | CD1 | TYR A | 36 | 42.927 | 53.383 | 16.454 | 1.00 | 14.21 | 6 |
| 234 | CB | LYS A | 31 | 32.771 | 56.667 | 7.818 | 1.00 | 13.99 | 6 | 276 | CD2 | TYR A | 36 | 43.807 | 52.460 | 14.391 | 1.00 | 16.88 | 6 |
| 235 | CG | LYS A | 31 | 31.981 | 57.980 | 8.050 | 1.00 | 13.23 | 6 | 277 | CE1 | TYR A | 36 | 43.317 | 52.206 | 17.122 | 1.00 | 14.97 | 6 |
| 236 | CD | LYS A | 31 | 30.617 | 57.569 | 8.669 | 1.00 | 16.17 | 6 | 278 | CE2 | TYR A | 36 | 44.182 | 51.320 | 15.075 | 1.00 | 19.02 | 6 |
| 237 | CE | LYS A | 31 | 29.763 | 58.766 | 9.053 | 1.00 | 14.65 | 6 | 279 | CZ | TYR A | 36 | 43.930 | 50.063 | 17.135 | 1.00 | 18.88 | 8 |
| 238 | NZ | LYS A | 31 | 30.427 | 59.568 | 10.156 | 1.00 | 12.05 | 7 | 280 | OH | TYR A | 36 | 44.299 | 50.063 | 17.135 | 1.00 | 18.88 | 8 |
| 239 | N | SER A | 32 | 35.822 | 57.610 | 8.364 | 1.00 | 16.27 | 7 | 281 | N | ASP A | 37 | 45.211 | 55.848 | 16.289 | 1.00 | 12.45 | 7 |
| 240 | CA | SER A | 32 | 36.675 | 58.587 | 9.038 | 1.00 | 14.39 | 6 | 282 | CA | ASP A | 37 | 46.646 | 55.624 | 16.621 | 1.00 | 12.80 | 6 |
| 241 | C | SER A | 32 | 38.087 | 57.989 | 9.161 | 1.00 | 17.62 | 6 | 283 | C | ASP A | 37 | 46.700 | 54.350 | 17.441 | 1.00 | 14.03 | 6 |
| 242 | O | SER A | 32 | 36.100 | 58.851 | 10.460 | 1.00 | 12.32 | 6 | 284 | O | ASP A | 37 | 46.507 | 54.281 | 18.673 | 1.00 | 13.32 | 8 |
| 243 | CB | SER A | 32 | 35.874 | 57.664 | 11.167 | 1.00 | 12.92 | 8 | 285 | CB | ASP A | 37 | 47.120 | 56.834 | 17.463 | 1.00 | 13.46 | 6 |
| 244 | OG | SER A | 32 | 38.596 | 57.524 | 8.010 | 1.00 | 14.71 | 7 | 286 | CG | ASP A | 37 | 48.543 | 56.543 | 17.991 | 1.00 | 20.57 | 6 |
| 245 | N | TYR A | 33 | 39.875 | 56.801 | 8.045 | 1.00 | 15.23 | 6 | 287 | OD1 | ASP A | 37 | 49.278 | 55.720 | 17.366 | 1.00 | 17.00 | 8 |
| 246 | CA | TYR A | 33 | 41.051 | 57.676 | 8.444 | 1.00 | 14.94 | 6 | 288 | OD2 | ASP A | 37 | 48.902 | 57.113 | 19.028 | 1.00 | 17.32 | 8 |
| 247 | C | TYR A | 33 | 41.042 | 58.848 | 8.023 | 1.00 | 17.62 | 8 | 289 | N | PRO A | 38 | 47.163 | 53.245 | 16.821 | 1.00 | 15.62 | 7 |
| 248 | O | TYR A | 33 | 40.075 | 56.295 | 6.582 | 1.00 | 18.09 | 6 | 290 | CA | PRO A | 38 | 47.375 | 52.024 | 17.548 | 1.00 | 15.67 | 6 |
| 249 | CB | TYR A | 33 | 41.166 | 55.254 | 6.536 | 1.00 | 20.46 | 6 | 291 | C | PRO A | 38 | 48.484 | 52.056 | 18.558 | 1.00 | 15.69 | 6 |
| 250 | CG | TYR A | 33 | 40.982 | 53.978 | 7.004 | 1.00 | 26.95 | 6 | 292 | O | PRO A | 38 | 48.513 | 51.189 | 19.436 | 1.00 | 18.95 | 8 |
| 251 | CD1 | TYR A | 33 | 42.408 | 55.618 | 6.002 | 1.00 | 31.14 | 6 | 293 | CB | PRO A | 38 | 47.669 | 50.946 | 16.450 | 1.00 | 17.01 | 6 |
| 252 | CD2 | TYR A | 33 | 41.994 | 53.027 | 6.944 | 1.00 | 33.56 | 6 | 294 | CG | PRO A | 38 | 48.367 | 51.843 | 15.437 | 1.00 | 18.68 | 6 |
| 253 | CE1 | TYR A | 33 | 43.422 | 54.670 | 5.943 | 1.00 | 31.30 | 6 | 295 | CD | PRO A | 38 | 47.570 | 53.192 | 15.409 | 1.00 | 18.22 | 6 |
| 254 | CE2 | TYR A | 33 | 43.210 | 53.409 | 6.402 | 1.00 | 33.88 | 6 | 296 | N | THR A | 39 | 49.385 | 53.031 | 18.514 | 1.00 | 15.60 | 7 |
| 255 | CZ | TYR A | 33 | 44.235 | 52.483 | 6.334 | 1.00 | 44.90 | 8 | 297 | CA | THR A | 39 | 50.469 | 53.080 | 19.499 | 1.00 | 14.85 | 6 |
| 256 | OH | TYR A | 33 | 42.039 | 57.105 | 9.114 | 1.00 | 12.92 | 7 | 298 | C | THR A | 39 | 50.126 | 53.773 | 20.822 | 1.00 | 17.68 | 6 |
| 257 | N | GLY A | 34 | 43.281 | 57.836 | 9.403 | 1.00 | 14.92 | 6 | 299 | O | THR A | 39 | 50.961 | 53.777 | 21.719 | 1.00 | 17.01 | 8 |
| 258 | CA | GLY A | 34 | 43.255 | 58.672 | 10.686 | 1.00 | 15.08 | 6 | 300 | CB | THR A | 39 | 51.692 | 53.847 | 18.947 | 1.00 | 19.14 | 6 |
| 259 | C | GLY A | 34 | 44.274 | 59.342 | 10.956 | 1.00 | 15.24 | 8 | 301 | OG1 | THR A | 39 | 51.503 | 55.239 | 18.723 | 1.00 | 16.66 | 8 |
| 260 | O | GLY A | 34 | 42.253 | 58.417 | 11.548 | 1.00 | 12.52 | 7 | 302 | CG2 | THR A | 39 | 52.083 | 53.233 | 17.573 | 1.00 | 22.20 | 6 |
| 261 | N | LEU A | 35 | 42.215 | 59.140 | 12.846 | 1.00 | 11.02 | 6 | 303 | N | LYS A | 40 | 48.983 | 54.487 | 20.832 | 1.00 | 14.93 | 7 |
| 262 | CA | LEU A | 35 | 42.519 | 58.271 | 14.028 | 1.00 | 15.01 | 6 | 304 | CA | LYS A | 40 | 48.588 | 55.225 | 22.041 | 1.00 | 14.22 | 6 |
| 263 | C | LEU A | 35 | | | | | | | 305 | C | LYS A | 40 | 49.736 | 56.141 | 22.483 | 1.00 | 17.80 | 6 |

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|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|--------|----|--------|--------|--------|------|-------|----|
| 306 | O | LYS A | 40 | 50.009 | 56.348 | 23.685 | 1.00 | 17.78 | 8 | 348 | CE | LYS A | 44 | 45.254 | 58.171 | 22.334 | 1.00 | 15.83 | 6 |
| 307 | CB | LYS A | 40 | 48.104 | 54.324 | 23.207 | 1.00 | 19.03 | 6 | 349 | NZ | LYS A | 44 | 45.125 | 69.681 | 22.068 | 1.00 | 18.92 | 7 |
| 308 | CG | LYS A | 40 | 47.023 | 53.320 | 22.775 | 1.00 | 18.65 | 6 | 350 | N | MET A | 45 | 44.473 | 61.576 | 19.114 | 1.00 | 10.42 | 7 |
| 309 | CD | LYS A | 40 | 46.535 | 52.543 | 24.031 | 1.00 | 21.38 | 6 | 351 | CA | MET A | 45 | 43.881 | 60.686 | 18.112 | 1.00 | 12.24 | 6 |
| 310 | CE | LYS A | 40 | 45.432 | 51.573 | 23.590 | 1.00 | 22.34 | 6 | 352 | C | MET A | 45 | 42.952 | 59.664 | 18.768 | 1.00 | 11.36 | 6 |
| 311 | NZ | LYS A | 40 | 45.883 | 50.563 | 22.605 | 1.00 | 21.85 | 7 | 353 | O | MET A | 45 | 43.011 | 59.512 | 19.985 | 1.00 | 12.88 | 8 |
| 312 | N | SER A | 41 | 50.307 | 56.831 | 21.475 | 1.00 | 16.33 | 7 | 354 | CB | MET A | 45 | 45.028 | 59.874 | 17.442 | 1.00 | 13.26 | 6 |
| 313 | CA | SER A | 41 | 51.307 | 57.853 | 21.746 | 1.00 | 17.21 | 6 | 355 | CG | AMET A | 45 | 46.067 | 60.710 | 16.692 | 0.50 | 14.78 | 6 |
| 314 | C | SER A | 41 | 50.929 | 59.210 | 21.203 | 1.00 | 16.87 | 6 | 356 | SD | AMET A | 45 | 45.379 | 61.237 | 15.135 | 0.50 | 13.95 | 16 |
| 315 | O | SER A | 41 | 51.606 | 60.250 | 21.492 | 1.00 | 16.04 | 8 | 357 | CE | AMET A | 45 | 45.728 | 60.040 | 13.903 | 0.50 | 12.41 | 6 |
| 316 | CB | SER A | 41 | 52.714 | 57.429 | 21.198 | 1.00 | 17.96 | 6 | 355 | CG | BMET A | 45 | 45.776 | 60.960 | 16.619 | 0.50 | 11.59 | 6 |
| 317 | OG | SER A | 41 | 52.625 | 57.387 | 19.782 | 1.00 | 20.42 | 8 | 356 | SD | BMET A | 45 | 46.918 | 60.290 | 15.431 | 0.50 | 16.20 | 16 |
| 318 | N | LYS A | 42 | 49.895 | 59.315 | 20.388 | 1.00 | 13.73 | 7 | 357 | CE | BMET A | 45 | 45.864 | 59.453 | 14.271 | 0.50 | 18.11 | 6 |
| 319 | CA | LYS A | 42 | 49.446 | 60.589 | 19.836 | 1.00 | 12.77 | 6 | 358 | N | TYR A | 46 | 42.122 | 58.961 | 17.976 | 1.00 | 10.91 | 7 |
| 320 | C | LYS A | 42 | 48.152 | 60.921 | 20.603 | 1.00 | 13.20 | 6 | 359 | CA | TYR A | 46 | 41.356 | 57.880 | 18.584 | 1.00 | 13.29 | 6 |
| 321 | O | LYS A | 42 | 47.111 | 60.351 | 20.317 | 1.00 | 12.98 | 8 | 360 | C | TYR A | 46 | 42.263 | 56.591 | 18.938 | 1.00 | 13.10 | 6 |
| 322 | CB | LYS A | 42 | 49.193 | 60.477 | 18.321 | 1.00 | 14.60 | 6 | 361 | O | TYR A | 46 | 43.076 | 56.318 | 18.094 | 1.00 | 12.46 | 8 |
| 323 | CG | LYS A | 42 | 50.523 | 60.079 | 17.606 | 1.00 | 19.41 | 6 | 362 | CB | TYR A | 46 | 40.258 | 57.364 | 17.660 | 1.00 | 12.44 | 6 |
| 324 | CD | LYS A | 42 | 50.228 | 60.163 | 16.078 | 1.00 | 25.03 | 6 | 363 | CG | TYR A | 46 | 39.031 | 58.210 | 17.416 | 1.00 | 13.02 | 6 |
| 325 | CE | LYS A | 42 | 51.611 | 60.340 | 15.395 | 1.00 | 34.65 | 6 | 364 | CD1 | TYR A | 46 | 39.075 | 59.210 | 16.436 | 1.00 | 11.30 | 6 |
| 326 | NZ | LYS A | 42 | 52.071 | 58.949 | 15.130 | 1.00 | 41.02 | 7 | 365 | CD2 | TYR A | 46 | 37.846 | 57.978 | 18.105 | 1.00 | 12.45 | 6 |
| 327 | N | TRP A | 43 | 48.256 | 61.858 | 21.565 | 1.00 | 11.08 | 7 | 366 | CE1 | TYR A | 46 | 37.940 | 59.997 | 16.146 | 1.00 | 12.75 | 6 |
| 328 | CA | TRP A | 43 | 47.235 | 61.925 | 22.643 | 1.00 | 13.35 | 6 | 367 | CE2 | TYR A | 46 | 36.683 | 58.746 | 17.838 | 1.00 | 9.77 | 6 |
| 329 | C | TRP A | 43 | 45.915 | 62.494 | 22.162 | 1.00 | 11.08 | 6 | 368 | CZ | TYR A | 46 | 36.789 | 59.707 | 16.881 | 1.00 | 10.60 | 6 |
| 330 | O | TRP A | 43 | 45.002 | 62.429 | 22.997 | 1.00 | 13.47 | 8 | 369 | OH | TYR A | 46 | 35.703 | 60.490 | 16.547 | 1.00 | 11.65 | 8 |
| 331 | CB | TRP A | 43 | 47.831 | 62.848 | 23.743 | 1.00 | 14.15 | 6 | 370 | N | TRP A | 47 | 42.097 | 56.222 | 20.188 | 1.00 | 9.67 | 7 |
| 332 | CG | TRP A | 43 | 48.739 | 61.957 | 24.592 | 1.00 | 12.91 | 6 | 371 | CA | TRP A | 47 | 42.866 | 55.089 | 20.664 | 1.00 | 11.50 | 6 |
| 333 | CD1 | TRP A | 43 | 50.014 | 61.590 | 24.338 | 1.00 | 14.88 | 6 | 372 | C | TRP A | 47 | 42.065 | 53.770 | 20.579 | 1.00 | 12.29 | 6 |
| 334 | CD2 | TRP A | 43 | 48.362 | 61.357 | 25.845 | 1.00 | 12.18 | 6 | 373 | O | TRP A | 47 | 42.633 | 52.676 | 20.711 | 1.00 | 12.20 | 8 |
| 335 | NE1 | TRP A | 43 | 50.507 | 60.770 | 25.364 | 1.00 | 16.61 | 7 | 374 | CB | TRP A | 47 | 43.430 | 55.285 | 22.077 | 1.00 | 12.80 | 6 |
| 336 | CE2 | TRP A | 43 | 49.467 | 60.633 | 26.297 | 1.00 | 17.08 | 6 | 375 | CG | TRP A | 47 | 44.548 | 56.316 | 22.086 | 1.00 | 10.46 | 6 |
| 337 | CE3 | TRP A | 43 | 47.186 | 61.367 | 26.617 | 1.00 | 13.97 | 6 | 376 | CD1 | TRP A | 47 | 45.068 | 57.007 | 21.037 | 1.00 | 11.88 | 6 |
| 338 | CZ2 | TRP A | 43 | 49.497 | 59.891 | 27.501 | 1.00 | 19.44 | 6 | 377 | CD2 | TRP A | 47 | 45.300 | 56.687 | 23.218 | 1.00 | 10.01 | 6 |
| 339 | CZ3 | TRP A | 43 | 47.223 | 60.644 | 27.814 | 1.00 | 14.34 | 6 | 378 | NE1 | TRP A | 47 | 46.060 | 57.853 | 21.485 | 1.00 | 11.36 | 7 |
| 340 | CH2 | TRP A | 43 | 48.333 | 59.925 | 28.265 | 1.00 | 15.92 | 6 | 379 | CE2 | TRP A | 47 | 46.219 | 57.700 | 22.820 | 1.00 | 12.07 | 6 |
| 341 | N | LYS A | 44 | 45.846 | 63.088 | 20.972 | 1.00 | 11.78 | 7 | 380 | CE3 | TRP A | 47 | 45.198 | 56.392 | 24.603 | 1.00 | 12.09 | 6 |
| 342 | CA | LYS A | 44 | 44.532 | 63.606 | 20.529 | 1.00 | 10.59 | 6 | 381 | CZ2 | TRP A | 47 | 47.103 | 58.301 | 23.715 | 1.00 | 13.05 | 6 |
| 343 | C | LYS A | 44 | 43.959 | 62.797 | 19.362 | 1.00 | 11.15 | 6 | 382 | CZ3 | TRP A | 47 | 46.072 | 56.974 | 25.484 | 1.00 | 15.07 | 6 |
| 344 | O | LYS A | 44 | 43.021 | 63.227 | 18.707 | 1.00 | 11.48 | 8 | 383 | CH2 | TRP A | 47 | 47.002 | 57.939 | 25.033 | 1.00 | 16.33 | 6 |
| 345 | CB | LYS A | 44 | 44.647 | 65.112 | 20.097 | 1.00 | 11.58 | 6 | 384 | N | GLY A | 48 | 40.752 | 53.875 | 20.442 | 1.00 | 10.96 | 7 |
| 346 | CG | LYS A | 44 | 45.053 | 65.911 | 21.382 | 1.00 | 11.48 | 6 | 385 | CA | GLY A | 48 | 39.995 | 52.631 | 20.097 | 1.00 | 11.53 | 6 |
| 347 | CD | LYS A | 44 | 44.928 | 67.435 | 21.011 | 1.00 | 12.19 | 6 | 386 | C | GLY A | 48 | 38.960 | 52.197 | 21.106 | 1.00 | 11.03 | 6 |

| | | | | | | | | | | | | | | | | | | | |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 387 | O | GLY A | 48 | 38.208 | 51.215 | 20.845 | 1.00 | 12.01 | 8 | 429 | CA | ARG A | 55 | 29.382 | 46.875 | 28.101 | 1.00 | 13.29 | 6 |
| 388 | N | GLY A | 49 | 38.834 | 52.862 | 22.221 | 1.00 | 12.42 | 7 | 430 | C | ARG A | 55 | 30.112 | 45.671 | 28.652 | 1.00 | 12.91 | 6 |
| 389 | CA | GLY A | 49 | 37.789 | 52.443 | 23.230 | 1.00 | 12.08 | 6 | 431 | O | ARG A | 55 | 29.684 | 44.943 | 29.596 | 1.00 | 13.96 | 8 |
| 390 | C | GLY A | 49 | 36.451 | 52.679 | 22.614 | 1.00 | 9.81 | 6 | 432 | CB | ARG A | 55 | 28.627 | 46.458 | 26.819 | 1.00 | 13.43 | 6 |
| 391 | O | GLY A | 49 | 36.173 | 53.629 | 21.880 | 1.00 | 10.92 | 8 | 433 | CG | ARG A | 55 | 27.364 | 45.611 | 27.165 | 1.00 | 13.64 | 6 |
| 392 | N | ASP A | 50 | 35.433 | 51.851 | 23.065 | 1.00 | 10.42 | 7 | 434 | CD | ARG A | 55 | 26.723 | 44.974 | 25.877 | 1.00 | 13.15 | 6 |
| 393 | CA | ASP A | 50 | 34.135 | 51.985 | 22.429 | 1.00 | 11.91 | 6 | 435 | NE | ARG A | 55 | 27.745 | 44.040 | 25.358 | 1.00 | 13.30 | 7 |
| 394 | C | ASP A | 50 | 32.977 | 51.516 | 23.344 | 1.00 | 11.85 | 6 | 436 | CE | ARG A | 55 | 28.117 | 42.905 | 25.921 | 1.00 | 14.35 | 6 |
| 395 | O | ASP A | 50 | 33.188 | 51.228 | 24.489 | 1.00 | 12.76 | 8 | 437 | NH1 | ARG A | 55 | 27.475 | 42.404 | 27.011 | 1.00 | 15.82 | 7 |
| 396 | CB | ASP A | 50 | 34.148 | 51.188 | 21.094 | 1.00 | 10.66 | 6 | 438 | NH2 | ARG A | 55 | 29.125 | 42.171 | 25.446 | 1.00 | 17.12 | 7 |
| 397 | CG | ASP A | 50 | 34.693 | 49.790 | 21.327 | 1.00 | 14.50 | 6 | 439 | N | GLN A | 56 | 31.265 | 45.354 | 28.031 | 1.00 | 11.75 | 7 |
| 398 | OD1 | ASP A | 50 | 34.446 | 49.184 | 22.384 | 1.00 | 11.19 | 8 | 440 | CA | GLN A | 56 | 32.050 | 44.171 | 28.503 | 1.00 | 12.69 | 6 |
| 399 | OD2 | ASP A | 50 | 35.425 | 49.205 | 20.532 | 1.00 | 11.87 | 8 | 441 | C | GLN A | 56 | 32.530 | 44.339 | 29.945 | 1.00 | 14.76 | 6 |
| 400 | N | LEU A | 51 | 31.762 | 51.615 | 22.778 | 1.00 | 11.80 | 7 | 442 | O | GLN A | 56 | 32.895 | 43.338 | 30.611 | 1.00 | 15.16 | 8 |
| 401 | CA | LEU A | 51 | 30.580 | 51.320 | 23.617 | 1.00 | 11.32 | 6 | 443 | CB | GLN A | 56 | 33.249 | 43.948 | 27.536 | 1.00 | 12.12 | 6 |
| 402 | C | LEU A | 51 | 30.568 | 49.843 | 23.973 | 1.00 | 13.43 | 6 | 444 | CG | GLN A | 56 | 32.718 | 43.310 | 26.223 | 1.00 | 12.45 | 6 |
| 403 | O | LEU A | 51 | 30.145 | 49.499 | 25.090 | 1.00 | 11.80 | 8 | 445 | CD | GLN A | 56 | 33.748 | 43.189 | 25.110 | 1.00 | 18.74 | 6 |
| 404 | CB | LEU A | 51 | 29.272 | 51.662 | 22.869 | 1.00 | 12.03 | 6 | 446 | OE1 | GLN A | 56 | 33.441 | 43.161 | 23.879 | 1.00 | 21.22 | 8 |
| 405 | CG | LEU A | 51 | 29.178 | 53.205 | 22.638 | 1.00 | 11.71 | 6 | 447 | NE2 | GLN A | 56 | 34.957 | 43.066 | 25.540 | 1.00 | 13.29 | 7 |
| 406 | CD1 | LEU A | 51 | 28.036 | 53.389 | 21.666 | 1.00 | 13.88 | 6 | 448 | N | LYS A | 57 | 32.816 | 45.574 | 30.355 | 1.00 | 13.93 | 7 |
| 407 | CD2 | LEU A | 51 | 28.915 | 53.930 | 23.954 | 1.00 | 15.76 | 6 | 449 | CA | LYS A | 57 | 33.243 | 45.881 | 31.703 | 1.00 | 11.77 | 6 |
| 408 | N | GLU A | 52 | 30.942 | 48.987 | 23.037 | 1.00 | 12.67 | 7 | 450 | C | LYS A | 57 | 32.146 | 46.200 | 32.702 | 1.00 | 13.05 | 6 |
| 409 | CA | GLU A | 52 | 30.995 | 47.541 | 23.443 | 1.00 | 12.25 | 6 | 451 | O | LYS A | 57 | 32.397 | 46.651 | 33.834 | 1.00 | 12.11 | 8 |
| 410 | C | GLU A | 52 | 32.024 | 47.239 | 24.516 | 1.00 | 12.73 | 6 | 452 | CB | LYS A | 57 | 34.240 | 47.112 | 31.625 | 1.00 | 12.27 | 6 |
| 411 | O | GLU A | 52 | 31.816 | 46.375 | 25.382 | 1.00 | 13.32 | 8 | 453 | CG | LYS A | 57 | 35.508 | 46.752 | 30.818 | 1.00 | 13.15 | 6 |
| 412 | CB | GLU A | 52 | 31.182 | 46.786 | 22.122 | 1.00 | 16.82 | 6 | 454 | CD | LYS A | 57 | 36.167 | 45.442 | 31.318 | 1.00 | 13.38 | 6 |
| 413 | CG | GLU A | 52 | 31.390 | 45.298 | 22.295 | 1.00 | 22.57 | 6 | 455 | CE | LYS A | 57 | 37.577 | 45.277 | 30.729 | 1.00 | 16.88 | 6 |
| 414 | CD | GLU A | 52 | 30.227 | 44.545 | 22.992 | 1.00 | 12.69 | 6 | 456 | NZ | LYS A | 57 | 38.170 | 43.960 | 31.261 | 1.00 | 17.21 | 7 |
| 415 | OE1 | GLU A | 52 | 29.097 | 45.029 | 23.005 | 1.00 | 17.98 | 8 | 457 | N | LEU A | 58 | 30.883 | 45.891 | 32.388 | 1.00 | 12.90 | 7 |
| 416 | OE2 | GLU A | 52 | 30.680 | 43.475 | 23.419 | 1.00 | 16.49 | 8 | 458 | CA | LEU A | 58 | 29.789 | 46.048 | 33.338 | 1.00 | 14.31 | 6 |
| 417 | N | GLY A | 53 | 33.114 | 48.012 | 24.628 | 1.00 | 12.03 | 7 | 459 | C | LEU A | 58 | 29.981 | 45.299 | 34.668 | 1.00 | 12.68 | 6 |
| 418 | CA | GLY A | 53 | 34.108 | 47.857 | 25.680 | 1.00 | 13.18 | 6 | 460 | O | LEU A | 58 | 29.737 | 45.865 | 35.732 | 1.00 | 13.94 | 8 |
| 419 | C | GLY A | 53 | 33.471 | 48.292 | 27.005 | 1.00 | 12.67 | 6 | 461 | CB | LEU A | 58 | 28.407 | 45.779 | 32.723 | 1.00 | 12.52 | 6 |
| 420 | O | GLY A | 53 | 33.737 | 47.586 | 28.000 | 1.00 | 11.91 | 8 | 462 | CG | LEU A | 58 | 27.963 | 46.878 | 31.718 | 1.00 | 12.14 | 6 |
| 421 | N | VAL A | 54 | 32.653 | 49.355 | 27.005 | 1.00 | 11.80 | 7 | 463 | CD1 | LEU A | 58 | 26.709 | 46.366 | 30.943 | 1.00 | 14.87 | 6 |
| 422 | CA | VAL A | 54 | 31.996 | 49.680 | 28.280 | 1.00 | 10.05 | 6 | 464 | CD2 | LEU A | 58 | 27.586 | 48.136 | 32.488 | 1.00 | 15.84 | 6 |
| 423 | C | VAL A | 54 | 31.078 | 48.502 | 28.715 | 1.00 | 12.37 | 6 | 465 | N | PRO A | 59 | 30.555 | 44.107 | 34.670 | 1.00 | 13.13 | 7 |
| 424 | O | VAL A | 54 | 31.055 | 48.111 | 29.879 | 1.00 | 12.15 | 8 | 466 | CA | PRO A | 59 | 30.776 | 43.396 | 35.937 | 1.00 | 14.64 | 6 |
| 425 | CB | VAL A | 54 | 31.154 | 50.947 | 28.220 | 1.00 | 11.03 | 6 | 467 | C | PRO A | 59 | 31.759 | 44.139 | 36.827 | 1.00 | 14.63 | 6 |
| 426 | CG1 | VAL A | 54 | 30.449 | 51.255 | 29.552 | 1.00 | 13.86 | 6 | 468 | O | PRO A | 59 | 31.532 | 44.250 | 38.038 | 1.00 | 15.79 | 8 |
| 427 | CG2 | VAL A | 54 | 32.100 | 52.143 | 27.853 | 1.00 | 11.86 | 6 | 469 | CB | PRO A | 59 | 31.436 | 42.034 | 35.525 | 1.00 | 15.40 | 6 |
| 428 | N | ARG A | 55 | 30.387 | 47.952 | 27.708 | 1.00 | 9.95 | 7 | 470 | CG | PRO A | 59 | 30.719 | 41.845 | 34.161 | 1.00 | 16.79 | 6 |

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|-----|-----------|--------|--------|--------|--------|--------|-------|-------|-----|---------|-----------|--------|--------|--------|--------|-------|-------|---|
| 471 | CD | PRO A | 59 | 30.807 | 43.247 | 33.514 | 1.00 | 16.71 | 6 | 508 | OE1BGLN A | 63 | 34.480 | 42.416 | 41.279 | 0.33 | 14.24 | 8 |
| 472 | N | TYR A | 60 | 32.806 | 44.717 | 36.210 | 1.00 | 12.89 | 7 | 509 | NE2BGLN A | 63 | 34.884 | 42.519 | 43.537 | 0.33 | 12.44 | 7 |
| 473 | CA | TYR A | 60 | 33.789 | 45.511 | 36.994 | 1.00 | 12.47 | 6 | 510 | N LEU A | 64 | 32.481 | 47.646 | 41.498 | 1.00 | 10.99 | 7 |
| 474 | C | TYR A | 60 | 33.072 | 46.731 | 37.584 | 1.00 | 12.64 | 6 | 511 | CA LEU A | 64 | 32.993 | 48.909 | 42.087 | 1.00 | 15.73 | 6 |
| 475 | O | TYR A | 60 | 33.237 | 46.994 | 38.797 | 1.00 | 13.63 | 8 | 512 | C LEU A | 64 | 31.893 | 49.656 | 42.837 | 1.00 | 14.21 | 6 |
| 476 | CB | TYR A | 60 | 34.918 | 45.920 | 36.026 | 1.00 | 12.16 | 6 | 513 | O LEU A | 64 | 32.253 | 50.516 | 43.659 | 1.00 | 14.81 | 8 |
| 477 | CG | TYR A | 60 | 35.856 | 46.938 | 36.667 | 1.00 | 12.17 | 6 | 514 | CB LEU A | 64 | 33.536 | 49.777 | 40.930 | 1.00 | 14.15 | 6 |
| 478 | CD1 | TYR A | 60 | 36.917 | 46.528 | 37.462 | 1.00 | 13.23 | 6 | 515 | CG LEU A | 64 | 34.050 | 51.201 | 41.274 | 1.00 | 13.04 | 6 |
| 479 | CD2 | TYR A | 60 | 35.602 | 48.293 | 36.453 | 1.00 | 12.24 | 6 | 516 | CD1 LEU A | 64 | 35.177 | 51.132 | 42.303 | 1.00 | 12.46 | 6 |
| 480 | CE1 | TYR A | 60 | 37.730 | 47.509 | 38.049 | 1.00 | 12.99 | 6 | 517 | CD2 LEU A | 64 | 34.587 | 51.825 | 39.963 | 1.00 | 12.70 | 6 |
| 481 | CE2 | TYR A | 60 | 36.438 | 49.268 | 37.022 | 1.00 | 14.93 | 6 | 518 | N GLY A | 65 | 30.605 | 49.492 | 42.566 | 1.00 | 14.23 | 7 |
| 482 | CZ | TYR A | 60 | 37.473 | 48.852 | 37.823 | 1.00 | 14.75 | 6 | 519 | CA GLY A | 65 | 29.537 | 50.247 | 43.205 | 1.00 | 13.78 | 6 |
| 483 | OH | TYR A | 60 | 38.287 | 49.782 | 38.464 | 1.00 | 13.93 | 8 | 520 | C GLY A | 65 | 28.987 | 51.337 | 42.311 | 1.00 | 14.56 | 6 |
| 484 | N | LEU A | 61 | 32.298 | 47.410 | 36.735 | 1.00 | 11.74 | 7 | 521 | O GLY A | 65 | 28.207 | 52.222 | 42.758 | 1.00 | 13.13 | 8 |
| 485 | CA | LEU A | 61 | 31.622 | 48.610 | 37.225 | 1.00 | 11.91 | 6 | 522 | N VAL A | 66 | 29.343 | 51.265 | 41.014 | 1.00 | 12.13 | 7 |
| 486 | C | LEU A | 61 | 30.570 | 48.316 | 38.272 | 1.00 | 14.11 | 6 | 523 | CA VAL A | 66 | 28.773 | 52.267 | 40.114 | 1.00 | 10.77 | 6 |
| 487 | O | LEU A | 61 | 30.508 | 49.022 | 39.283 | 1.00 | 13.33 | 8 | 524 | C VAL A | 66 | 27.297 | 52.007 | 39.842 | 1.00 | 13.82 | 6 |
| 488 | CB | LEU A | 61 | 30.993 | 49.382 | 36.051 | 1.00 | 12.06 | 6 | 525 | O VAL A | 66 | 26.933 | 50.836 | 39.617 | 1.00 | 13.38 | 8 |
| 489 | CG | LEU A | 61 | 32.030 | 49.809 | 34.992 | 1.00 | 13.18 | 6 | 526 | CB VAL A | 66 | 29.491 | 52.192 | 38.744 | 1.00 | 11.10 | 6 |
| 490 | CD1 | LEU A | 61 | 31.263 | 50.310 | 33.753 | 1.00 | 15.35 | 6 | 527 | CG1 VAL A | 66 | 28.892 | 53.220 | 37.731 | 1.00 | 12.12 | 6 |
| 491 | CD2 | LEU A | 61 | 32.865 | 50.971 | 35.605 | 1.00 | 16.34 | 6 | 528 | CG2 VAL A | 66 | 30.961 | 52.489 | 38.974 | 1.00 | 14.48 | 6 |
| 492 | N | LYS A | 62 | 29.850 | 47.217 | 38.162 | 1.00 | 12.47 | 7 | 529 | N THR A | 67 | 26.431 | 53.016 | 39.992 | 1.00 | 10.70 | 7 |
| 493 | CA | LYS A | 62 | 28.890 | 46.844 | 39.202 | 1.00 | 13.25 | 6 | 530 | CA THR A | 67 | 25.022 | 52.822 | 39.675 | 1.00 | 12.22 | 6 |
| 494 | C | LYS A | 62 | 29.614 | 46.558 | 40.535 | 1.00 | 13.60 | 6 | 531 | C THR A | 67 | 24.526 | 53.737 | 38.565 | 1.00 | 13.77 | 6 |
| 495 | O | LYS A | 62 | 29.149 | 47.032 | 41.576 | 1.00 | 15.97 | 8 | 532 | O THR A | 67 | 23.404 | 53.538 | 38.103 | 1.00 | 13.29 | 8 |
| 496 | CB | LYS A | 62 | 28.117 | 45.588 | 38.730 | 1.00 | 14.71 | 6 | 533 | CB THR A | 67 | 24.072 | 52.926 | 40.898 | 1.00 | 14.25 | 6 |
| 497 | CG | LYS A | 62 | 27.011 | 45.263 | 39.764 | 1.00 | 17.27 | 6 | 534 | OG1 THR A | 67 | 24.680 | 53.791 | 41.874 | 1.00 | 13.89 | 8 |
| 498 | CD | LYS A | 62 | 25.908 | 44.363 | 39.223 | 1.00 | 30.17 | 6 | 535 | CG2 THR A | 67 | 24.085 | 51.519 | 41.584 | 1.00 | 14.96 | 6 |
| 499 | CE | LYS A | 62 | 24.879 | 44.088 | 40.343 | 1.00 | 25.52 | 6 | 536 | N THR A | 68 | 25.351 | 54.723 | 38.156 | 1.00 | 12.63 | 7 |
| 500 | NZ | LYS A | 62 | 23.887 | 45.203 | 40.515 | 1.00 | 24.63 | 7 | 537 | CA THR A | 68 | 25.042 | 55.479 | 36.914 | 1.00 | 10.68 | 6 |
| 501 | N | GLN A | 63 | 30.722 | 45.781 | 40.455 | 1.00 | 12.05 | 7 | 538 | C THR A | 68 | 26.379 | 55.684 | 36.193 | 1.00 | 9.37 | 6 |
| 502 | CA | GLN A | 63 | 31.437 | 45.448 | 41.660 | 1.00 | 10.80 | 6 | 539 | O THR A | 68 | 27.313 | 56.214 | 36.775 | 1.00 | 11.86 | 8 |
| 503 | C | GLN A | 63 | 32.010 | 46.705 | 42.325 | 1.00 | 13.71 | 6 | 540 | CB THR A | 68 | 24.388 | 56.837 | 37.236 | 1.00 | 13.89 | 6 |
| 504 | O | GLN A | 63 | 32.200 | 46.751 | 43.544 | 1.00 | 13.66 | 8 | 541 | OG1 THR A | 68 | 23.094 | 56.649 | 37.793 | 1.00 | 13.19 | 8 |
| 505 | CB | AGLN A | 63 | 32.582 | 44.501 | 41.262 | 0.66 | 17.93 | 6 | 542 | CG2 THR A | 68 | 24.269 | 57.734 | 35.965 | 1.00 | 14.32 | 6 |
| 506 | CG | AGLN A | 63 | 32.178 | 43.092 | 40.865 | 0.66 | 27.01 | 6 | 543 | N ILE A | 69 | 26.394 | 55.287 | 34.896 | 1.00 | 9.42 | 7 |
| 507 | CD | AGLN A | 63 | 33.421 | 42.362 | 40.343 | 0.66 | 35.95 | 6 | 544 | CA ILE A | 69 | 27.605 | 55.600 | 34.073 | 1.00 | 8.17 | 6 |
| 508 | OE1AGLN A | 63 | 34.283 | 42.022 | 41.149 | 0.66 | 40.99 | 8 | 545 | C ILE A | 69 | 27.249 | 56.897 | 33.377 | 1.00 | 11.16 | 6 | |
| 509 | NE2AGLN A | 63 | 33.525 | 42.128 | 39.043 | 0.66 | 36.04 | 7 | 546 | O ILE A | 69 | 26.200 | 57.080 | 32.734 | 1.00 | 12.50 | 8 | |
| 505 | CB | BGLN A | 63 | 32.511 | 44.387 | 41.345 | 0.33 | 7.59 | 6 | 547 | CB ILE A | 69 | 27.714 | 54.510 | 32.986 | 1.00 | 12.66 | 6 |
| 506 | CG | BGLN A | 63 | 33.072 | 43.793 | 42.621 | 0.33 | 8.29 | 6 | 548 | CG1 ILE A | 69 | 28.160 | 53.214 | 33.736 | 1.00 | 14.05 | 6 |
| 507 | CD | BGLN A | 63 | 34.234 | 42.824 | 42.408 | 0.33 | 8.28 | 6 | 549 | CG2 ILE A | 69 | 28.737 | 54.893 | 31.900 | 1.00 | 11.22 | 6 |

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|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| 550 | CD1 | ILE | A | 69 | 27.937 | 52.008 | 32.775 | 1.00 | 13.93 | 6 | 592 | CG2 | VAL | A | 74 | 25.882 | 58.894 | 22.161 | 1.00 | 10.26 | 6 |
| 551 | N | TRP | A | 70 | 28.196 | 57.872 | 33.425 | 1.00 | 9.74 | 7 | 593 | N | LEU | A | 75 | 27.708 | 60.912 | 19.980 | 1.00 | 10.62 | 7 |
| 552 | CA | TRP | A | 70 | 28.095 | 59.093 | 32.600 | 1.00 | 10.34 | 6 | 594 | CA | LEU | A | 75 | 27.182 | 61.136 | 18.619 | 1.00 | 10.48 | 6 |
| 553 | C | TRP | A | 70 | 28.991 | 58.790 | 31.403 | 1.00 | 11.63 | 6 | 595 | C | LEU | A | 75 | 28.305 | 61.464 | 17.620 | 1.00 | 12.02 | 6 |
| 554 | O | TRP | A | 70 | 30.214 | 58.751 | 31.558 | 1.00 | 11.51 | 8 | 596 | O | LEU | A | 75 | 29.436 | 61.678 | 18.016 | 1.00 | 11.28 | 8 |
| 555 | CB | TRP | A | 70 | 28.494 | 60.327 | 33.441 | 1.00 | 9.83 | 6 | 597 | CB | LEU | A | 75 | 26.111 | 62.279 | 18.660 | 1.00 | 10.81 | 6 |
| 556 | CG | TRP | A | 70 | 28.954 | 61.558 | 32.738 | 1.00 | 8.81 | 6 | 598 | CG | LEU | A | 75 | 24.952 | 61.966 | 19.634 | 1.00 | 11.49 | 6 |
| 557 | CD1 | TRP | A | 70 | 29.050 | 61.770 | 31.360 | 1.00 | 13.03 | 6 | 599 | CD1 | LEU | A | 75 | 24.074 | 63.178 | 19.911 | 1.00 | 11.47 | 6 |
| 558 | CD2 | TRP | A | 70 | 29.591 | 62.698 | 33.356 | 1.00 | 10.57 | 6 | 600 | CD2 | LEU | A | 75 | 24.074 | 60.864 | 18.960 | 1.00 | 11.05 | 6 |
| 559 | NE1 | TRP | A | 70 | 29.645 | 63.016 | 31.118 | 1.00 | 12.41 | 7 | 601 | N | ASP | A | 76 | 27.958 | 61.296 | 16.347 | 1.00 | 10.11 | 7 |
| 560 | CE2 | TRP | A | 70 | 30.017 | 63.558 | 32.338 | 1.00 | 10.48 | 6 | 602 | CA | ASP | A | 76 | 29.020 | 61.292 | 15.299 | 1.00 | 9.23 | 6 |
| 561 | CE3 | TRP | A | 70 | 29.830 | 63.007 | 34.699 | 1.00 | 12.18 | 6 | 603 | C | ASP | A | 76 | 29.821 | 62.605 | 15.351 | 1.00 | 9.60 | 6 |
| 562 | C22 | TRP | A | 70 | 30.721 | 64.729 | 32.587 | 1.00 | 9.61 | 6 | 604 | O | ASP | A | 76 | 29.263 | 63.683 | 15.155 | 1.00 | 11.11 | 8 |
| 563 | C23 | TRP | A | 70 | 30.426 | 64.234 | 34.950 | 1.00 | 11.62 | 6 | 605 | CB | ASP | A | 76 | 28.264 | 61.153 | 13.979 | 1.00 | 9.89 | 6 |
| 564 | CH2 | TRP | A | 70 | 30.896 | 65.061 | 33.914 | 1.00 | 13.98 | 6 | 606 | CG | ASP | A | 76 | 29.177 | 61.079 | 12.745 | 1.00 | 12.56 | 6 |
| 565 | N | LEU | A | 71 | 28.373 | 58.542 | 30.225 | 1.00 | 10.83 | 7 | 607 | OD1 | ASP | A | 76 | 30.380 | 60.856 | 12.895 | 1.00 | 12.97 | 8 |
| 566 | CA | LEU | A | 71 | 29.219 | 58.311 | 29.023 | 1.00 | 11.92 | 6 | 608 | OD2 | ASP | A | 76 | 28.617 | 61.239 | 11.641 | 1.00 | 11.97 | 8 |
| 567 | C | LEU | A | 71 | 29.585 | 59.691 | 28.439 | 1.00 | 10.49 | 6 | 609 | N | ASN | A | 77 | 31.131 | 62.435 | 15.524 | 1.00 | 9.80 | 7 |
| 568 | O | LEU | A | 71 | 28.669 | 60.552 | 28.276 | 1.00 | 10.64 | 8 | 610 | CA | ASN | A | 77 | 32.043 | 63.570 | 15.534 | 1.00 | 9.86 | 6 |
| 569 | CB | LEU | A | 71 | 28.342 | 57.617 | 27.923 | 1.00 | 11.13 | 6 | 611 | C | ASN | A | 77 | 32.766 | 63.691 | 14.180 | 1.00 | 10.69 | 6 |
| 570 | CG | LEU | A | 71 | 27.991 | 56.159 | 28.240 | 1.00 | 11.31 | 6 | 612 | O | ASN | A | 77 | 32.797 | 62.759 | 13.385 | 1.00 | 10.51 | 8 |
| 571 | CD1 | LEU | A | 71 | 27.073 | 55.665 | 27.096 | 1.00 | 10.98 | 6 | 613 | CB | ASN | A | 77 | 33.117 | 63.370 | 16.619 | 1.00 | 10.13 | 6 |
| 572 | CD2 | LEU | A | 71 | 29.253 | 55.314 | 28.322 | 1.00 | 11.96 | 6 | 614 | CG | ASN | A | 77 | 32.685 | 63.988 | 17.945 | 1.00 | 13.40 | 6 |
| 573 | N | SER | A | 72 | 30.870 | 59.865 | 28.066 | 1.00 | 10.17 | 7 | 615 | OD1 | ASN | A | 77 | 33.515 | 64.636 | 18.600 | 1.00 | 10.92 | 8 |
| 574 | CA | SER | A | 72 | 31.250 | 60.995 | 27.218 | 1.00 | 9.81 | 6 | 616 | ND2 | ASN | A | 77 | 31.412 | 63.908 | 18.341 | 1.00 | 11.73 | 7 |
| 575 | C | SER | A | 72 | 30.455 | 60.988 | 25.920 | 1.00 | 11.22 | 6 | 617 | N | LEU | A | 78 | 33.296 | 64.886 | 13.967 | 1.00 | 10.62 | 7 |
| 576 | O | SER | A | 72 | 29.733 | 60.011 | 25.572 | 1.00 | 10.33 | 8 | 618 | CA | LEU | A | 78 | 34.240 | 65.195 | 12.866 | 1.00 | 11.24 | 6 |
| 577 | CB | SER | A | 72 | 32.773 | 60.898 | 26.944 | 1.00 | 10.62 | 6 | 619 | C | LEU | A | 78 | 34.929 | 63.977 | 12.309 | 1.00 | 8.87 | 6 |
| 578 | CG | SER | A | 72 | 33.092 | 59.694 | 26.237 | 1.00 | 11.62 | 8 | 620 | O | LEU | A | 78 | 35.632 | 63.257 | 13.026 | 1.00 | 12.04 | 8 |
| 579 | N | PRO | A | 73 | 30.447 | 62.034 | 25.128 | 1.00 | 11.10 | 7 | 621 | CB | LEU | A | 78 | 35.257 | 66.197 | 13.506 | 1.00 | 9.81 | 6 |
| 580 | CA | PRO | A | 73 | 29.427 | 62.188 | 24.048 | 1.00 | 11.86 | 6 | 622 | CG | LEU | A | 78 | 36.289 | 66.679 | 12.399 | 1.00 | 9.30 | 6 |
| 581 | C | PRO | A | 73 | 29.521 | 61.057 | 23.042 | 1.00 | 13.54 | 6 | 623 | CD1 | LEU | A | 78 | 35.622 | 67.597 | 11.418 | 1.00 | 11.34 | 6 |
| 582 | O | PRO | A | 73 | 30.653 | 60.649 | 22.674 | 1.00 | 11.75 | 8 | 624 | CD2 | LEU | A | 78 | 37.382 | 67.439 | 13.176 | 1.00 | 13.04 | 6 |
| 583 | CB | PRO | A | 73 | 29.672 | 63.563 | 23.414 | 1.00 | 10.32 | 6 | 625 | N | ASP | A | 79 | 34.801 | 63.867 | 10.945 | 1.00 | 11.36 | 7 |
| 584 | CG | PRO | A | 73 | 30.360 | 64.313 | 24.557 | 1.00 | 10.23 | 6 | 626 | CA | ASP | A | 79 | 35.393 | 62.670 | 10.348 | 1.00 | 9.32 | 6 |
| 585 | CD | PRO | A | 73 | 31.228 | 63.286 | 25.358 | 1.00 | 11.09 | 6 | 627 | C | ASP | A | 79 | 36.754 | 62.947 | 9.688 | 1.00 | 12.70 | 6 |
| 586 | N | VAL | A | 74 | 28.345 | 60.538 | 22.623 | 1.00 | 11.02 | 7 | 628 | O | ASP | A | 79 | 37.275 | 62.042 | 9.026 | 1.00 | 14.30 | 8 |
| 587 | CA | VAL | A | 74 | 28.351 | 59.338 | 21.794 | 1.00 | 9.14 | 6 | 629 | CB | ASP | A | 79 | 34.468 | 62.189 | 9.168 | 1.00 | 14.19 | 6 |
| 588 | C | VAL | A | 74 | 27.998 | 59.628 | 20.344 | 1.00 | 9.79 | 6 | 630 | CG | ASP | A | 79 | 33.217 | 61.518 | 9.658 | 1.00 | 15.14 | 6 |
| 589 | O | VAL | A | 74 | 28.041 | 58.700 | 19.549 | 1.00 | 10.96 | 8 | 631 | OD1 | ASP | A | 79 | 33.208 | 61.150 | 10.841 | 1.00 | 12.50 | 8 |
| 590 | CB | VAL | A | 74 | 27.260 | 58.313 | 22.311 | 1.00 | 9.29 | 6 | 632 | OD2 | ASP | A | 79 | 32.239 | 61.307 | 8.931 | 1.00 | 12.26 | 8 |
| 591 | CG1 | VAL | A | 74 | 27.541 | 57.935 | 23.780 | 1.00 | 11.66 | 6 | 633 | N | THR | A | 80 | 37.307 | 64.115 | 9.950 | 1.00 | 12.57 | 7 |

| | | | | | | | | | | | | | | | | | | | |
|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| 634 | CA | THR A | 80 | 38.652 | 64.479 | 9.456 | 1.00 | 14.13 | 6 | 676 | CB | ASN A | 86 | 44.190 | 67.732 | 16.468 | 1.00 | 11.52 | 6 |
| 635 | C | THR A | 80 | 39.521 | 64.930 | 10.635 | 1.00 | 13.16 | 6 | 677 | CB | ASN A | 86 | 43.470 | 68.295 | 17.677 | 1.00 | 13.68 | 6 |
| 636 | O | THR A | 80 | 39.072 | 64.981 | 11.769 | 1.00 | 12.58 | 8 | 678 | OD1 | ASN A | 86 | 42.743 | 67.535 | 18.341 | 1.00 | 14.08 | 8 |
| 637 | CB | THR A | 80 | 38.583 | 65.712 | 8.534 | 1.00 | 14.19 | 6 | 679 | ND2 | ASN A | 86 | 43.644 | 69.546 | 18.063 | 1.00 | 15.21 | 7 |
| 638 | OG1 | THR A | 80 | 38.265 | 66.927 | 9.264 | 1.00 | 15.46 | 8 | 680 | N | THR A | 87 | 41.877 | 65.099 | 16.705 | 1.00 | 10.11 | 7 |
| 639 | CG2 | THR A | 80 | 37.593 | 65.645 | 7.372 | 1.00 | 19.78 | 6 | 681 | CA | THR A | 87 | 40.619 | 64.459 | 16.251 | 1.00 | 10.70 | 6 |
| 640 | N | LEU A | 81 | 40.809 | 65.216 | 10.327 | 1.00 | 13.37 | 7 | 682 | C | THR A | 87 | 39.525 | 64.643 | 17.317 | 1.00 | 11.84 | 6 |
| 641 | CA | LEU A | 81 | 41.651 | 65.864 | 11.341 | 1.00 | 10.22 | 6 | 683 | O | THR A | 87 | 39.764 | 65.021 | 18.471 | 1.00 | 11.11 | 8 |
| 642 | C | LEU A | 81 | 41.263 | 67.297 | 11.488 | 1.00 | 12.10 | 6 | 684 | CB | THR A | 87 | 40.745 | 62.924 | 16.124 | 1.00 | 12.30 | 6 |
| 643 | O | LEU A | 81 | 40.635 | 67.900 | 10.595 | 1.00 | 12.72 | 8 | 685 | OG1 | THR A | 87 | 40.840 | 62.298 | 17.444 | 1.00 | 11.34 | 8 |
| 644 | CB | LEU A | 81 | 43.143 | 65.818 | 10.830 | 1.00 | 10.42 | 6 | 686 | CG2 | THR A | 87 | 41.961 | 62.467 | 15.375 | 1.00 | 11.19 | 6 |
| 645 | CG | LEU A | 81 | 43.643 | 64.345 | 10.809 | 1.00 | 15.27 | 6 | 687 | N | GLY A | 88 | 38.307 | 64.357 | 16.903 | 1.00 | 11.28 | 7 |
| 646 | CD1 | LEU A | 81 | 44.897 | 64.351 | 9.927 | 1.00 | 21.14 | 6 | 688 | CA | GLY A | 88 | 37.184 | 64.329 | 17.887 | 1.00 | 10.27 | 6 |
| 647 | CD2 | LEU A | 81 | 44.059 | 63.885 | 12.244 | 1.00 | 14.05 | 6 | 689 | C | GLY A | 88 | 37.107 | 63.063 | 18.721 | 1.00 | 10.54 | 6 |
| 648 | N | ALA A | 82 | 41.647 | 67.888 | 12.629 | 1.00 | 11.74 | 7 | 690 | O | GLY A | 88 | 35.954 | 62.712 | 19.121 | 1.00 | 10.21 | 8 |
| 649 | CA | ALA A | 82 | 41.548 | 69.320 | 12.798 | 1.00 | 13.34 | 6 | 691 | N | TYR A | 89 | 38.196 | 62.404 | 19.087 | 1.00 | 10.33 | 7 |
| 650 | C | ALA A | 82 | 42.941 | 69.801 | 13.202 | 1.00 | 12.91 | 6 | 692 | CA | TYR A | 89 | 38.134 | 61.241 | 19.955 | 1.00 | 10.06 | 6 |
| 651 | O | ALA A | 82 | 43.208 | 70.247 | 14.316 | 1.00 | 11.11 | 8 | 693 | C | TYR A | 89 | 37.314 | 61.476 | 21.204 | 1.00 | 11.70 | 6 |
| 652 | CB | ALA A | 82 | 40.566 | 69.586 | 13.989 | 1.00 | 14.40 | 6 | 694 | O | TYR A | 89 | 36.760 | 60.489 | 21.732 | 1.00 | 11.42 | 8 |
| 653 | N | GLY A | 83 | 43.811 | 69.835 | 12.180 | 1.00 | 12.89 | 7 | 695 | CB | TYR A | 89 | 39.564 | 60.769 | 20.316 | 1.00 | 9.10 | 6 |
| 654 | CA | GLY A | 83 | 45.245 | 70.145 | 12.484 | 1.00 | 11.52 | 6 | 696 | CG | TYR A | 89 | 40.152 | 61.653 | 21.412 | 1.00 | 11.07 | 6 |
| 655 | C | GLY A | 83 | 45.960 | 68.860 | 12.923 | 1.00 | 12.02 | 6 | 697 | CD1 | TYR A | 89 | 40.732 | 62.857 | 21.106 | 1.00 | 10.61 | 6 |
| 656 | O | GLY A | 83 | 45.405 | 67.737 | 13.060 | 1.00 | 11.47 | 8 | 698 | CD2 | TYR A | 89 | 40.058 | 61.256 | 22.750 | 1.00 | 9.12 | 6 |
| 657 | N | THR A | 84 | 47.262 | 68.987 | 13.230 | 1.00 | 12.31 | 7 | 699 | CE1 | TYR A | 89 | 41.243 | 63.688 | 22.115 | 1.00 | 9.21 | 6 |
| 658 | CA | THR A | 84 | 48.160 | 67.879 | 13.444 | 1.00 | 11.91 | 6 | 700 | CE2 | TYR A | 89 | 40.505 | 62.054 | 23.777 | 1.00 | 11.90 | 6 |
| 659 | C | THR A | 84 | 47.716 | 66.883 | 14.496 | 1.00 | 10.74 | 6 | 701 | CZ | TYR A | 89 | 41.098 | 63.267 | 23.443 | 1.00 | 10.92 | 6 |
| 660 | O | THR A | 84 | 47.554 | 67.213 | 15.687 | 1.00 | 11.33 | 8 | 702 | OH | TYR A | 89 | 41.593 | 64.126 | 24.411 | 1.00 | 10.82 | 8 |
| 661 | CB | THR A | 84 | 49.570 | 68.477 | 13.888 | 1.00 | 10.32 | 6 | 703 | N | HIS A | 90 | 37.283 | 62.703 | 21.748 | 1.00 | 10.85 | 7 |
| 662 | OG1 | THR A | 84 | 49.942 | 69.432 | 12.873 | 1.00 | 12.17 | 8 | 704 | CA | HIS A | 90 | 36.623 | 62.983 | 23.011 | 1.00 | 9.54 | 6 |
| 663 | CG2 | THR A | 84 | 50.533 | 67.298 | 14.074 | 1.00 | 13.58 | 6 | 705 | C | HIS A | 90 | 35.095 | 63.104 | 22.837 | 1.00 | 7.69 | 6 |
| 664 | N | ASP A | 85 | 47.462 | 65.652 | 14.019 | 1.00 | 12.06 | 7 | 706 | O | HIS A | 90 | 34.392 | 63.040 | 23.856 | 1.00 | 9.02 | 8 |
| 665 | CA | ASP A | 85 | 47.117 | 64.552 | 14.933 | 1.00 | 10.80 | 6 | 707 | CB | HIS A | 90 | 37.178 | 64.338 | 23.555 | 1.00 | 10.73 | 6 |
| 666 | C | ASP A | 85 | 45.981 | 64.902 | 15.894 | 1.00 | 12.31 | 6 | 708 | CG | HIS A | 90 | 37.294 | 65.403 | 22.507 | 1.00 | 11.48 | 6 |
| 667 | O | ASP A | 85 | 45.986 | 64.416 | 17.030 | 1.00 | 13.43 | 8 | 709 | ND1 | HIS A | 90 | 36.210 | 66.035 | 21.926 | 1.00 | 9.73 | 7 |
| 668 | CB | ASP A | 85 | 48.356 | 64.077 | 15.747 | 1.00 | 14.44 | 6 | 710 | CD2 | HIS A | 90 | 38.405 | 65.898 | 21.906 | 1.00 | 8.93 | 6 |
| 669 | CG | ASP A | 85 | 49.500 | 63.600 | 14.831 | 1.00 | 22.31 | 6 | 711 | CE1 | HIS A | 90 | 36.686 | 66.903 | 21.010 | 1.00 | 10.94 | 6 |
| 670 | OD1 | ASP A | 85 | 49.284 | 63.065 | 13.744 | 1.00 | 14.91 | 8 | 712 | NE2 | HIS A | 90 | 37.988 | 66.862 | 20.995 | 1.00 | 10.18 | 7 |
| 671 | OD2 | ASP A | 85 | 50.645 | 63.782 | 15.275 | 1.00 | 23.25 | 8 | 713 | N | GLY A | 91 | 34.616 | 63.356 | 21.629 | 1.00 | 9.66 | 7 |
| 672 | N | ASN A | 86 | 45.024 | 65.712 | 15.418 | 1.00 | 10.53 | 7 | 714 | CA | GLY A | 91 | 33.143 | 63.393 | 21.404 | 1.00 | 9.79 | 6 |
| 673 | CA | ASN A | 86 | 44.024 | 66.196 | 16.401 | 1.00 | 10.12 | 6 | 715 | C | GLY A | 91 | 32.505 | 64.768 | 21.395 | 1.00 | 10.82 | 6 |
| 674 | C | ASN A | 86 | 42.644 | 65.784 | 15.880 | 1.00 | 9.75 | 6 | 716 | O | GLY A | 91 | 31.287 | 64.916 | 21.102 | 1.00 | 11.09 | 8 |
| 675 | O | ASN A | 86 | 42.241 | 66.073 | 14.747 | 1.00 | 12.30 | 8 | 717 | N | TYR A | 92 | 33.288 | 65.840 | 21.633 | 1.00 | 10.15 | 7 |

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|-----|-----|-------|----|--------|--------|--------|------|-------|---|-----|-----------|-----|--------|--------|--------|------|-------|---|
| 718 | CA | TYR A | 92 | 32.653 | 67.152 | 21.753 | 1.00 | 10.44 | 6 | 760 | NH2 ARG A | 95 | 30.477 | 64.026 | 7.380 | 1.00 | 15.12 | 7 |
| 719 | C | TYR A | 92 | 32.556 | 67.935 | 20.459 | 1.00 | 8.85 | 6 | 761 | N ASP A | 96 | 26.880 | 65.176 | 13.503 | 1.00 | 11.44 | 7 |
| 720 | O | TYR A | 92 | 32.132 | 69.141 | 20.520 | 1.00 | 9.64 | 8 | 762 | CA ASP A | 96 | 25.536 | 64.640 | 13.218 | 1.00 | 11.75 | 6 |
| 721 | CB | TYR A | 92 | 33.461 | 67.977 | 22.837 | 1.00 | 10.08 | 6 | 763 | C ASP A | 96 | 24.977 | 64.166 | 14.570 | 1.00 | 10.37 | 6 |
| 722 | CG | TYR A | 92 | 33.217 | 67.385 | 24.219 | 1.00 | 10.98 | 6 | 764 | O ASP A | 96 | 25.448 | 63.154 | 15.091 | 1.00 | 12.67 | 8 |
| 723 | CD1 | TYR A | 92 | 32.091 | 67.719 | 24.974 | 1.00 | 10.25 | 6 | 765 | CB ASP A | 96 | 25.622 | 63.467 | 12.217 | 1.00 | 10.69 | 6 |
| 724 | CD2 | TYR A | 92 | 34.112 | 66.472 | 24.730 | 1.00 | 10.46 | 6 | 766 | CG ASP A | 96 | 24.238 | 63.012 | 11.732 | 1.00 | 14.77 | 6 |
| 725 | CE1 | TYR A | 92 | 31.905 | 67.143 | 26.247 | 1.00 | 10.96 | 6 | 767 | OD1 ASP A | 96 | 23.229 | 63.251 | 12.412 | 1.00 | 11.10 | 8 |
| 726 | CE2 | TYR A | 92 | 33.932 | 65.888 | 25.983 | 1.00 | 14.14 | 6 | 768 | OD2 ASP A | 96 | 24.218 | 62.343 | 10.551 | 1.00 | 15.82 | 8 |
| 727 | CZ | TYR A | 92 | 32.829 | 66.237 | 26.715 | 1.00 | 11.56 | 6 | 769 | N PHE A | 97 | 24.007 | 64.989 | 15.033 | 1.00 | 9.84 | 7 |
| 728 | OH | TYR A | 92 | 32.648 | 65.665 | 27.970 | 1.00 | 12.31 | 8 | 770 | CA PHE A | 97 | 23.482 | 64.615 | 16.377 | 1.00 | 10.91 | 6 |
| 729 | N | TRP A | 93 | 32.968 | 67.343 | 19.345 | 1.00 | 10.19 | 7 | 771 | C PHE A | 97 | 22.504 | 63.426 | 16.336 | 1.00 | 13.19 | 6 |
| 730 | CA | TRP A | 93 | 32.914 | 68.040 | 18.039 | 1.00 | 11.73 | 6 | 772 | O PHE A | 97 | 21.945 | 63.125 | 17.373 | 1.00 | 13.15 | 8 |
| 731 | C | TRP A | 93 | 31.949 | 67.307 | 17.103 | 1.00 | 9.84 | 6 | 773 | CB PHE A | 97 | 22.818 | 65.844 | 16.982 | 1.00 | 10.58 | 6 |
| 732 | O | TRP A | 93 | 32.336 | 66.443 | 16.294 | 1.00 | 10.83 | 8 | 774 | CG PHE A | 97 | 23.783 | 66.935 | 17.422 | 1.00 | 14.29 | 6 |
| 733 | CB | TRP A | 93 | 34.322 | 68.024 | 17.415 | 1.00 | 12.42 | 6 | 775 | CD1 PHE A | 97 | 24.438 | 67.807 | 16.532 | 1.00 | 13.03 | 6 |
| 734 | CG | TRP A | 93 | 35.359 | 68.775 | 18.253 | 1.00 | 11.75 | 6 | 776 | CD2 PHE A | 97 | 23.979 | 67.062 | 18.799 | 1.00 | 13.39 | 6 |
| 735 | CD1 | TRP A | 93 | 35.181 | 69.659 | 19.258 | 1.00 | 12.58 | 6 | 777 | CE1 PHE A | 97 | 25.321 | 68.786 | 17.067 | 1.00 | 11.37 | 6 |
| 736 | CD2 | TRP A | 93 | 36.786 | 68.657 | 18.020 | 1.00 | 11.96 | 6 | 778 | CE2 PHE A | 97 | 24.780 | 68.073 | 19.296 | 1.00 | 9.92 | 6 |
| 737 | NE1 | TRP A | 93 | 36.448 | 70.120 | 19.694 | 1.00 | 13.60 | 7 | 779 | CZ PHE A | 97 | 25.489 | 68.930 | 18.467 | 1.00 | 9.67 | 6 |
| 738 | CE2 | TRP A | 93 | 37.397 | 69.501 | 18.932 | 1.00 | 14.78 | 6 | 780 | N LYS A | 98 | 22.220 | 62.889 | 15.152 | 1.00 | 11.59 | 7 |
| 739 | CE3 | TRP A | 93 | 37.559 | 67.884 | 17.130 | 1.00 | 13.74 | 6 | 781 | CA LYS A | 98 | 21.249 | 61.786 | 15.105 | 1.00 | 10.99 | 6 |
| 740 | CZ2 | TRP A | 93 | 38.808 | 69.626 | 19.040 | 1.00 | 15.96 | 6 | 782 | C LYS A | 98 | 21.893 | 60.424 | 14.982 | 1.00 | 13.58 | 6 |
| 741 | CZ3 | TRP A | 93 | 38.959 | 68.021 | 17.209 | 1.00 | 10.95 | 6 | 783 | O LYS A | 98 | 21.136 | 59.437 | 14.991 | 1.00 | 14.00 | 8 |
| 742 | CH2 | TRP A | 93 | 39.526 | 68.880 | 18.171 | 1.00 | 9.91 | 6 | 784 | CB LYS A | 98 | 20.375 | 61.999 | 13.835 | 1.00 | 10.72 | 6 |
| 743 | N | THR A | 94 | 30.669 | 67.534 | 17.237 | 1.00 | 10.45 | 7 | 785 | CG LYS A | 98 | 19.595 | 63.337 | 13.915 | 1.00 | 11.63 | 6 |
| 744 | CA | THR A | 94 | 29.603 | 66.690 | 16.661 | 1.00 | 9.91 | 6 | 786 | CD LYS A | 98 | 18.627 | 63.408 | 15.091 | 1.00 | 16.21 | 6 |
| 745 | C | THR A | 94 | 29.244 | 67.242 | 15.270 | 1.00 | 11.32 | 6 | 787 | CE LYS A | 98 | 17.808 | 64.707 | 15.036 | 1.00 | 16.03 | 6 |
| 746 | O | THR A | 94 | 28.854 | 68.415 | 15.074 | 1.00 | 11.48 | 8 | 788 | NZ LYS A | 98 | 16.876 | 64.605 | 13.828 | 1.00 | 15.90 | 7 |
| 747 | CB | THR A | 94 | 28.302 | 66.837 | 17.495 | 1.00 | 9.85 | 6 | 789 | N GLN A | 99 | 23.233 | 60.336 | 14.853 | 1.00 | 9.90 | 7 |
| 748 | OG1 | THR A | 94 | 28.643 | 66.563 | 18.891 | 1.00 | 11.49 | 8 | 790 | CA GLN A | 99 | 23.900 | 59.079 | 14.613 | 1.00 | 11.53 | 6 |
| 749 | CG2 | THR A | 94 | 27.263 | 65.739 | 17.079 | 1.00 | 11.23 | 6 | 791 | C GLN A | 99 | 25.042 | 58.866 | 15.625 | 1.00 | 12.11 | 6 |
| 750 | N | ARG A | 95 | 29.315 | 66.299 | 14.292 | 1.00 | 10.33 | 7 | 792 | O GLN A | 99 | 25.610 | 59.842 | 16.118 | 1.00 | 13.41 | 8 |
| 751 | CA | ARG A | 95 | 28.819 | 66.623 | 12.945 | 1.00 | 11.51 | 6 | 793 | CB GLN A | 99 | 24.657 | 58.975 | 13.225 | 1.00 | 13.31 | 6 |
| 752 | C | ARG A | 95 | 27.382 | 66.123 | 12.703 | 1.00 | 13.19 | 6 | 794 | CG GLN A | 99 | 23.575 | 58.962 | 12.137 | 1.00 | 20.81 | 6 |
| 753 | O | ARG A | 95 | 26.834 | 66.523 | 11.700 | 1.00 | 12.00 | 8 | 795 | CD GLN A | 99 | 24.005 | 57.830 | 11.187 | 1.00 | 47.61 | 6 |
| 754 | CB | ARG A | 95 | 29.766 | 65.999 | 11.920 | 1.00 | 12.95 | 6 | 796 | OE1 GLN A | 99 | 23.966 | 56.639 | 11.540 | 1.00 | 38.44 | 8 |
| 755 | CG | ARG A | 95 | 29.739 | 64.437 | 11.900 | 1.00 | 9.03 | 6 | 797 | NE2 GLN A | 99 | 24.435 | 58.330 | 10.031 | 1.00 | 51.18 | 7 |
| 756 | CD | ARG A | 95 | 30.894 | 63.964 | 11.008 | 1.00 | 12.99 | 6 | 798 | N ILE A | 100 | 25.139 | 57.581 | 16.003 | 1.00 | 11.97 | 7 |
| 757 | NE | ARG A | 95 | 30.917 | 64.346 | 9.584 | 1.00 | 13.10 | 7 | 799 | CA ILE A | 100 | 26.265 | 57.291 | 16.916 | 1.00 | 9.69 | 6 |
| 758 | CZ | ARG A | 95 | 30.216 | 63.680 | 8.633 | 1.00 | 13.74 | 6 | 800 | C ILE A | 100 | 27.586 | 57.395 | 16.160 | 1.00 | 11.29 | 6 |
| 759 | NH1 | ARG A | 95 | 29.307 | 62.746 | 8.918 | 1.00 | 13.30 | 7 | 801 | O ILE A | 100 | 27.744 | 57.032 | 14.974 | 1.00 | 13.58 | 8 |

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|-----|-----|-----------|--------|--------|--------|------------|---|-----|-----|-----------|--------|--------|--------|------------|---|
| 802 | CB | ILE A 100 | 26.080 | 55.834 | 17.385 | 1.00 11.20 | 6 | 844 | CZ | PHE A 104 | 34.365 | 58.005 | 21.053 | 1.00 13.46 | 6 |
| 803 | CG1 | ILE A 100 | 24.767 | 55.651 | 18.197 | 1.00 13.05 | 6 | 845 | N | GLY A 105 | 30.491 | 52.584 | 17.759 | 1.00 14.42 | 7 |
| 804 | CG2 | ILE A 100 | 27.229 | 55.284 | 18.240 | 1.00 10.14 | 6 | 846 | CA | GLY A 105 | 29.462 | 51.533 | 17.546 | 1.00 16.52 | 6 |
| 805 | CD1 | ILE A 100 | 24.692 | 56.541 | 19.489 | 1.00 13.82 | 6 | 847 | C | GLY A 105 | 28.362 | 52.143 | 16.670 | 1.00 17.63 | 6 |
| 806 | N | GLU A 101 | 28.607 | 57.861 | 16.898 | 1.00 11.66 | 7 | 848 | O | GLY A 105 | 28.624 | 53.104 | 15.927 | 1.00 14.43 | 8 |
| 807 | CA | GLU A 101 | 29.968 | 57.886 | 16.332 | 1.00 11.19 | 6 | 849 | N | ASN A 106 | 27.169 | 51.558 | 16.664 | 1.00 14.15 | 7 |
| 808 | C | GLU A 101 | 30.443 | 56.478 | 15.956 | 1.00 11.88 | 6 | 850 | CA | ASN A 106 | 26.017 | 52.150 | 15.960 | 1.00 11.27 | 6 |
| 809 | O | GLU A 101 | 30.430 | 55.545 | 16.758 | 1.00 12.38 | 8 | 851 | C | ASN A 106 | 24.864 | 52.149 | 16.958 | 1.00 13.27 | 6 |
| 810 | CB | GLU A 101 | 30.918 | 58.478 | 17.400 | 1.00 11.53 | 6 | 852 | O | ASN A 106 | 25.081 | 51.890 | 18.174 | 1.00 13.00 | 8 |
| 811 | CG | GLU A 101 | 32.427 | 58.256 | 17.126 | 1.00 10.12 | 6 | 853 | CB | ASN A 106 | 25.756 | 51.332 | 14.677 | 1.00 13.55 | 6 |
| 812 | CD | GLU A 101 | 32.796 | 58.791 | 15.715 | 1.00 10.82 | 6 | 854 | CG | ASN A 106 | 25.465 | 49.876 | 14.958 | 1.00 18.28 | 6 |
| 813 | OE1 | GLU A 101 | 32.328 | 59.903 | 15.389 | 1.00 11.74 | 8 | 855 | OD1 | ASN A 106 | 25.093 | 49.459 | 16.033 | 1.00 17.05 | 8 |
| 814 | OE2 | GLU A 101 | 33.577 | 58.059 | 15.099 | 1.00 12.29 | 8 | 856 | ND2 | ASN A 106 | 25.576 | 49.021 | 13.910 | 1.00 22.96 | 7 |
| 815 | N | GLU A 102 | 30.874 | 56.411 | 14.662 | 1.00 12.51 | 7 | 857 | N | TRP A 107 | 23.668 | 52.508 | 16.525 | 1.00 12.62 | 7 |
| 816 | CA | GLU A 102 | 31.192 | 55.081 | 14.116 | 1.00 11.29 | 6 | 858 | CA | TRP A 107 | 22.554 | 52.559 | 17.465 | 1.00 13.67 | 6 |
| 817 | C | GLU A 102 | 32.387 | 54.443 | 14.766 | 1.00 12.50 | 6 | 859 | C | TRP A 107 | 22.296 | 51.203 | 18.121 | 1.00 14.10 | 6 |
| 818 | O | GLU A 102 | 32.460 | 53.176 | 14.813 | 1.00 11.57 | 8 | 860 | O | TRP A 107 | 21.827 | 51.121 | 19.274 | 1.00 14.66 | 8 |
| 819 | CB | GLU A 102 | 31.402 | 55.182 | 12.553 | 1.00 11.80 | 6 | 861 | CB | TRP A 107 | 21.268 | 53.087 | 16.802 | 1.00 14.53 | 6 |
| 820 | CG | GLU A 102 | 32.656 | 55.982 | 12.107 | 1.00 12.52 | 6 | 862 | CG | TRP A 107 | 21.256 | 54.576 | 16.836 | 1.00 16.29 | 6 |
| 821 | CD | GLU A 102 | 32.465 | 57.475 | 12.181 | 1.00 12.69 | 6 | 863 | CD1 | TRP A 107 | 21.351 | 55.357 | 15.696 | 1.00 17.56 | 6 |
| 822 | OE1 | GLU A 102 | 31.368 | 58.018 | 12.431 | 1.00 14.09 | 8 | 864 | CD2 | TRP A 107 | 21.131 | 55.454 | 17.949 | 1.00 15.71 | 6 |
| 823 | OE2 | GLU A 102 | 33.493 | 58.174 | 11.930 | 1.00 15.94 | 8 | 865 | NE1 | TRP A 107 | 21.279 | 56.677 | 16.088 | 1.00 16.73 | 7 |
| 824 | N | HIS A 103 | 33.391 | 55.145 | 15.324 | 1.00 9.73 | 7 | 866 | CE2 | TRP A 107 | 21.186 | 56.759 | 17.451 | 1.00 14.24 | 6 |
| 825 | CA | HIS A 103 | 34.429 | 54.494 | 16.120 | 1.00 9.99 | 6 | 867 | CE3 | TRP A 107 | 20.995 | 55.256 | 19.345 | 1.00 13.30 | 6 |
| 826 | C | HIS A 103 | 33.862 | 53.874 | 17.376 | 1.00 11.88 | 6 | 868 | CE2 | TRP A 107 | 21.082 | 57.915 | 18.240 | 1.00 14.74 | 6 |
| 827 | O | HIS A 103 | 34.531 | 52.943 | 17.864 | 1.00 12.86 | 8 | 869 | CE3 | TRP A 107 | 20.919 | 56.410 | 20.131 | 1.00 16.80 | 6 |
| 828 | CB | HIS A 103 | 35.470 | 55.578 | 16.584 | 1.00 12.93 | 6 | 870 | CH2 | TRP A 107 | 20.927 | 57.717 | 19.596 | 1.00 13.00 | 6 |
| 829 | CG | HIS A 103 | 36.364 | 56.049 | 15.481 | 1.00 11.28 | 6 | 871 | N | THR A 108 | 22.439 | 50.097 | 17.351 | 1.00 14.29 | 7 |
| 830 | ND1 | HIS A 103 | 36.015 | 57.085 | 14.639 | 1.00 12.54 | 7 | 872 | CA | THR A 108 | 22.316 | 48.792 | 18.020 | 1.00 14.34 | 6 |
| 831 | CD2 | HIS A 103 | 37.595 | 55.655 | 15.123 | 1.00 14.43 | 6 | 873 | C | THR A 108 | 23.305 | 48.617 | 19.154 | 1.00 16.18 | 6 |
| 832 | CE1 | HIS A 103 | 37.021 | 57.288 | 13.749 | 1.00 13.58 | 6 | 874 | O | THR A 108 | 22.945 | 48.095 | 20.224 | 1.00 14.57 | 8 |
| 833 | NE2 | HIS A 103 | 37.965 | 56.434 | 14.054 | 1.00 13.95 | 7 | 875 | CB | THR A 108 | 22.508 | 47.669 | 16.969 | 1.00 16.38 | 6 |
| 834 | N | PHE A 104 | 32.662 | 54.253 | 17.819 | 1.00 9.60 | 7 | 876 | CG1 | THR A 108 | 21.473 | 47.841 | 16.005 | 1.00 18.39 | 8 |
| 835 | CA | PHE A 104 | 32.171 | 53.727 | 19.103 | 1.00 10.30 | 6 | 877 | CG2 | THR A 108 | 22.386 | 46.276 | 17.600 | 1.00 20.41 | 6 |
| 836 | C | PHE A 104 | 31.116 | 52.625 | 18.924 | 1.00 13.76 | 6 | 878 | N | THR A 109 | 24.581 | 49.043 | 18.959 | 1.00 12.36 | 7 |
| 837 | O | PHE A 104 | 30.969 | 51.851 | 19.894 | 1.00 13.23 | 8 | 879 | CA | THR A 109 | 25.556 | 48.897 | 20.029 | 1.00 13.35 | 6 |
| 838 | CB | PHE A 104 | 31.583 | 54.855 | 19.953 | 1.00 10.00 | 6 | 880 | C | THR A 109 | 25.149 | 49.732 | 21.248 | 1.00 12.11 | 6 |
| 839 | CG | PHE A 104 | 32.587 | 55.933 | 20.330 | 1.00 11.59 | 6 | 881 | O | THR A 109 | 25.318 | 49.282 | 22.382 | 1.00 12.78 | 8 |
| 840 | CD1 | PHE A 104 | 33.954 | 55.782 | 20.204 | 1.00 11.92 | 6 | 882 | CB | THR A 109 | 26.960 | 49.404 | 19.545 | 1.00 13.85 | 6 |
| 841 | CD2 | PHE A 104 | 32.082 | 57.130 | 20.834 | 1.00 13.49 | 6 | 883 | CG1 | THR A 109 | 27.201 | 49.021 | 18.155 | 1.00 14.22 | 8 |
| 842 | CE1 | PHE A 104 | 34.854 | 56.802 | 20.561 | 1.00 12.32 | 6 | 884 | CG2 | THR A 109 | 28.048 | 48.783 | 20.429 | 1.00 15.14 | 6 |
| 843 | CE2 | PHE A 104 | 32.981 | 58.161 | 21.193 | 1.00 11.48 | 6 | 885 | N | PHE A 110 | 24.673 | 50.945 | 20.982 | 1.00 12.96 | 7 |

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|-----|-----|-----------|--------|--------|--------|------------|---|-----|-----|-----------|--------|--------|--------|------------|---|
| 886 | CA | PHE A 110 | 24.247 | 51.800 | 22.126 | 1.00 12.43 | 6 | 928 | C | ASN A 115 | 20.678 | 46.553 | 28.961 | 1.00 12.99 | 6 |
| 887 | C | PHE A 110 | 23.058 | 51.137 | 22.830 | 1.00 13.48 | 6 | 929 | O | ASN A 115 | 20.121 | 46.160 | 29.987 | 1.00 15.11 | 8 |
| 888 | O | PHE A 110 | 23.061 | 51.036 | 24.060 | 1.00 12.36 | 8 | 930 | CB | ASN A 115 | 19.372 | 46.637 | 26.820 | 1.00 15.99 | 6 |
| 889 | CB | PHE A 110 | 23.823 | 53.160 | 21.525 | 1.00 14.28 | 6 | 931 | CG | ASN A 115 | 18.200 | 47.261 | 26.118 | 1.00 22.41 | 6 |
| 890 | CG | PHE A 110 | 23.320 | 54.128 | 22.611 | 1.00 15.08 | 6 | 932 | OD1 | ASN A 115 | 18.061 | 47.131 | 24.868 | 1.00 26.38 | 8 |
| 891 | CD1 | PHE A 110 | 24.190 | 54.941 | 23.252 | 1.00 13.29 | 6 | 933 | ND2 | ASN A 115 | 17.304 | 47.937 | 26.823 | 1.00 22.30 | 7 |
| 892 | CD2 | PHE A 110 | 21.975 | 54.202 | 22.913 | 1.00 14.29 | 6 | 934 | N | ASP A 116 | 21.940 | 46.229 | 28.669 | 1.00 12.94 | 7 |
| 893 | CE1 | PHE A 110 | 23.764 | 55.850 | 24.247 | 1.00 13.20 | 6 | 935 | CA | ASP A 116 | 22.731 | 45.386 | 29.561 | 1.00 12.20 | 6 |
| 894 | CE2 | PHE A 110 | 21.487 | 55.055 | 23.876 | 1.00 12.89 | 6 | 936 | C | ASP A 116 | 23.087 | 46.144 | 30.835 | 1.00 12.69 | 6 |
| 895 | CZ | PHE A 110 | 22.377 | 55.898 | 24.558 | 1.00 13.20 | 6 | 937 | O | ASP A 116 | 23.070 | 45.584 | 31.933 | 1.00 12.40 | 8 |
| 896 | N | ASP A 111 | 22.056 | 50.645 | 22.065 | 1.00 13.15 | 7 | 938 | CB | ASP A 116 | 23.989 | 44.814 | 28.887 | 1.00 13.19 | 6 |
| 897 | CA | ASP A 111 | 20.916 | 49.993 | 22.755 | 1.00 12.63 | 6 | 939 | CG | ASP A 116 | 23.648 | 43.698 | 27.896 | 1.00 19.33 | 6 |
| 898 | C | ASP A 111 | 21.337 | 48.770 | 23.517 | 1.00 14.08 | 6 | 940 | OD1 | ASP A 116 | 22.461 | 43.487 | 27.582 | 1.00 23.80 | 8 |
| 899 | O | ASP A 111 | 20.917 | 48.606 | 24.698 | 1.00 14.41 | 8 | 941 | OD2 | ASP A 116 | 24.583 | 42.967 | 27.460 | 1.00 22.90 | 8 |
| 900 | CB | ASP A 111 | 19.966 | 49.513 | 21.610 | 1.00 13.40 | 6 | 942 | N | ALA A 117 | 23.342 | 47.453 | 30.753 | 1.00 12.25 | 7 |
| 901 | CG | ASP A 111 | 19.224 | 50.603 | 20.937 | 1.00 18.96 | 6 | 943 | CA | ALA A 117 | 23.561 | 48.208 | 32.005 | 1.00 12.13 | 6 |
| 902 | OD1 | ASP A 111 | 19.343 | 51.768 | 21.305 | 1.00 17.72 | 8 | 944 | C | ALA A 117 | 22.314 | 48.146 | 32.878 | 1.00 10.66 | 6 |
| 903 | OD2 | ASP A 111 | 18.498 | 50.291 | 19.945 | 1.00 18.78 | 8 | 945 | O | ALA A 117 | 22.425 | 47.887 | 34.083 | 1.00 12.92 | 8 |
| 904 | N | THR A 112 | 22.284 | 48.006 | 22.997 | 1.00 13.38 | 7 | 946 | CB | ALA A 117 | 23.877 | 49.692 | 31.625 | 1.00 13.05 | 6 |
| 905 | CA | THR A 112 | 22.756 | 46.828 | 23.718 | 1.00 14.87 | 6 | 947 | N | HIS A 118 | 21.149 | 48.403 | 32.291 | 1.00 12.02 | 7 |
| 906 | C | THR A 112 | 23.450 | 47.184 | 25.017 | 1.00 14.48 | 6 | 948 | CA | HIS A 118 | 19.948 | 48.334 | 33.131 | 1.00 10.66 | 6 |
| 907 | O | THR A 112 | 23.224 | 46.583 | 26.069 | 1.00 15.04 | 8 | 949 | C | HIS A 118 | 19.727 | 46.929 | 33.683 | 1.00 12.65 | 6 |
| 908 | CB | THR A 112 | 23.680 | 45.966 | 22.829 | 1.00 15.99 | 6 | 950 | O | HIS A 118 | 19.267 | 46.870 | 34.838 | 1.00 14.87 | 8 |
| 909 | OG1 | THR A 112 | 22.844 | 45.644 | 21.711 | 1.00 16.67 | 8 | 951 | CB | HIS A 118 | 18.714 | 48.622 | 32.200 | 1.00 10.79 | 6 |
| 910 | CG2 | THR A 112 | 24.006 | 44.662 | 23.576 | 1.00 18.86 | 6 | 952 | CG | HIS A 118 | 18.691 | 50.088 | 31.789 | 1.00 11.37 | 6 |
| 911 | N | LEU A 113 | 24.321 | 48.221 | 24.968 | 1.00 11.85 | 7 | 953 | ND1 | HIS A 118 | 17.881 | 50.557 | 30.773 | 1.00 14.86 | 7 |
| 912 | CA | LEU A 113 | 24.982 | 48.631 | 26.219 | 1.00 12.44 | 6 | 954 | CD2 | HIS A 118 | 19.340 | 51.157 | 32.359 | 1.00 13.69 | 6 |
| 913 | C | LEU A 113 | 23.992 | 49.138 | 27.242 | 1.00 12.26 | 6 | 955 | CE1 | HIS A 118 | 18.020 | 51.897 | 30.708 | 1.00 15.91 | 6 |
| 914 | O | LEU A 113 | 24.057 | 48.793 | 28.403 | 1.00 12.86 | 8 | 956 | NE2 | HIS A 118 | 18.912 | 52.260 | 31.644 | 1.00 11.99 | 7 |
| 915 | CB | LEU A 113 | 25.988 | 49.772 | 25.811 | 1.00 10.14 | 6 | 957 | N | GLN A 119 | 20.028 | 45.871 | 32.935 | 1.00 11.93 | 7 |
| 916 | CG | LEU A 113 | 26.404 | 50.629 | 27.037 | 1.00 13.26 | 6 | 958 | CA | GLN A 119 | 19.843 | 44.545 | 33.592 | 1.00 12.22 | 6 |
| 917 | CD1 | LEU A 113 | 27.184 | 49.772 | 28.040 | 1.00 13.59 | 6 | 959 | C | GLN A 119 | 20.770 | 44.412 | 34.781 | 1.00 15.02 | 6 |
| 918 | CD2 | LEU A 113 | 27.295 | 51.825 | 26.664 | 1.00 12.75 | 6 | 960 | O | GLN A 119 | 20.519 | 43.615 | 35.694 | 1.00 15.33 | 8 |
| 919 | N | VAL A 114 | 23.020 | 49.971 | 26.823 | 1.00 11.82 | 7 | 961 | CB | GLN A 119 | 20.340 | 43.445 | 32.620 | 1.00 16.20 | 6 |
| 920 | CA | VAL A 114 | 22.073 | 50.545 | 27.762 | 1.00 12.84 | 6 | 962 | CG | GLN A 119 | 19.327 | 43.169 | 31.521 | 1.00 17.09 | 6 |
| 921 | C | VAL A 114 | 21.215 | 49.449 | 28.384 | 1.00 13.48 | 6 | 963 | CD | GLN A 119 | 20.028 | 41.969 | 30.765 | 1.00 21.33 | 6 |
| 922 | O | VAL A 114 | 20.973 | 49.402 | 29.577 | 1.00 13.54 | 8 | 964 | OE1 | GLN A 119 | 20.575 | 41.051 | 31.363 | 1.00 29.71 | 8 |
| 923 | CB | VAL A 114 | 21.264 | 51.680 | 27.090 | 1.00 13.71 | 6 | 965 | NE2 | GLN A 119 | 19.985 | 42.085 | 29.522 | 1.00 20.93 | 7 |
| 924 | CG1 | VAL A 114 | 20.144 | 52.091 | 28.032 | 1.00 18.18 | 6 | 966 | N | ASN A 120 | 21.939 | 45.127 | 34.806 | 1.00 15.33 | 7 |
| 925 | CG2 | VAL A 114 | 22.209 | 52.885 | 26.815 | 1.00 15.06 | 6 | 967 | CA | ASN A 120 | 22.853 | 45.072 | 35.932 | 1.00 16.39 | 6 |
| 926 | N | ASN A 115 | 20.760 | 48.534 | 27.512 | 1.00 13.50 | 7 | 968 | C | ASN A 120 | 22.541 | 46.148 | 36.970 | 1.00 14.25 | 6 |
| 927 | CA | ASN A 115 | 19.912 | 47.430 | 28.013 | 1.00 11.60 | 6 | 969 | O | ASN A 120 | 23.358 | 46.337 | 37.876 | 1.00 15.65 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|-----------------|
| 970 | CB | ASN A 120 | 24.337 | 45.189 | 35.481 | 1.00 | 12.26 | 6 | 1012 | C | VAL A 126 | 25.247 | 62.207 | 28.081 | 1.00 | 12.61 | 6 |
| 971 | CG | ASN A 120 | 24.753 | 43.901 | 34.799 | 1.00 | 20.80 | 6 | 1013 | O | VAL A 126 | 24.413 | 63.080 | 28.254 | 1.00 | 11.41 | 8 |
| 972 | OD1 | ASN A 120 | 24.778 | 43.805 | 33.576 | 1.00 | 23.34 | 8 | 1014 | CB | VAL A 126 | 24.039 | 60.356 | 26.823 | 1.00 | 11.44 | 6 |
| 973 | ND2 | ASN A 120 | 25.076 | 42.912 | 35.627 | 1.00 | 18.29 | 7 | 1015 | CG1 | VAL A 126 | 24.892 | 60.704 | 25.575 | 1.00 | 12.92 | 6 |
| 974 | N | GLY A 121 | 21.398 | 46.801 | 36.951 | 1.00 | 13.35 | 7 | 1016 | CG2 | VAL A 126 | 23.704 | 58.883 | 26.856 | 1.00 | 11.52 | 6 |
| 975 | CA | GLY A 121 | 20.994 | 47.834 | 37.885 | 1.00 | 16.91 | 6 | 1017 | N | ASP A 127 | 26.535 | 62.445 | 27.771 | 1.00 | 8.46 | 7 |
| 976 | C | GLY A 121 | 21.840 | 49.129 | 37.772 | 1.00 | 13.99 | 6 | 1018 | CA | ASP A 127 | 27.011 | 63.870 | 27.661 | 1.00 | 9.67 | 6 |
| 977 | O | GLY A 121 | 21.866 | 49.890 | 38.747 | 1.00 | 15.35 | 8 | 1019 | C | ASP A 127 | 26.509 | 64.374 | 26.283 | 1.00 | 10.71 | 6 |
| 978 | N | ILE A 122 | 22.262 | 49.397 | 36.527 | 1.00 | 12.67 | 7 | 1020 | O | ASP A 127 | 26.837 | 63.710 | 25.279 | 1.00 | 11.36 | 8 |
| 979 | CA | ILE A 122 | 23.128 | 50.569 | 36.322 | 1.00 | 13.01 | 6 | 1021 | CB | ASP A 127 | 28.552 | 63.719 | 27.694 | 1.00 | 9.91 | 6 |
| 980 | C | ILE A 122 | 22.464 | 51.454 | 35.289 | 1.00 | 13.96 | 6 | 1022 | CG | ASP A 127 | 29.305 | 64.951 | 28.135 | 1.00 | 11.94 | 6 |
| 981 | O | ILE A 122 | 22.075 | 50.945 | 34.227 | 1.00 | 12.86 | 8 | 1023 | OD1 | ASP A 127 | 28.822 | 66.041 | 27.747 | 1.00 | 11.17 | 8 |
| 982 | CB | ILE A 122 | 24.556 | 50.129 | 35.886 | 1.00 | 12.06 | 6 | 1024 | OD2 | ASP A 127 | 30.335 | 64.880 | 28.865 | 1.00 | 10.63 | 8 |
| 983 | CG1 | ILE A 122 | 25.320 | 49.424 | 37.040 | 1.00 | 15.35 | 6 | 1025 | N | PHE A 128 | 25.802 | 65.484 | 26.325 | 1.00 | 8.41 | 7 |
| 984 | CG2 | ILE A 122 | 25.415 | 51.348 | 35.506 | 1.00 | 13.36 | 6 | 1026 | CA | PHE A 128 | 25.134 | 65.952 | 25.077 | 1.00 | 9.40 | 6 |
| 985 | CD1 | ILE A 122 | 26.569 | 48.709 | 36.465 | 1.00 | 15.31 | 6 | 1027 | C | PHE A 128 | 25.609 | 67.394 | 24.887 | 1.00 | 9.48 | 6 |
| 986 | N | LYS A 123 | 22.344 | 52.752 | 35.609 | 1.00 | 11.45 | 7 | 1028 | O | PHE A 128 | 25.752 | 68.163 | 25.858 | 1.00 | 10.67 | 8 |
| 987 | CA | LYS A 123 | 21.767 | 53.718 | 34.652 | 1.00 | 11.74 | 6 | 1029 | CB | PHE A 128 | 23.609 | 66.006 | 25.437 | 1.00 | 9.59 | 6 |
| 988 | C | LYS A 123 | 22.865 | 54.362 | 33.786 | 1.00 | 11.74 | 6 | 1030 | CG | PHE A 128 | 22.760 | 66.405 | 24.223 | 1.00 | 8.93 | 6 |
| 989 | O | LYS A 123 | 24.052 | 54.129 | 34.057 | 1.00 | 11.17 | 8 | 1031 | CD1 | PHE A 128 | 22.719 | 65.597 | 23.104 | 1.00 | 12.26 | 6 |
| 990 | CB | LYS A 123 | 21.051 | 54.811 | 35.457 | 1.00 | 11.34 | 6 | 1032 | CD2 | PHE A 128 | 22.095 | 67.627 | 24.315 | 1.00 | 10.12 | 6 |
| 991 | CG | LYS A 123 | 19.832 | 54.205 | 36.163 | 1.00 | 12.23 | 6 | 1033 | CE1 | PHE A 128 | 21.907 | 66.014 | 22.027 | 1.00 | 12.04 | 6 ^{UN} |
| 992 | CD | LYS A 123 | 18.994 | 55.310 | 36.815 | 1.00 | 16.30 | 6 | 1034 | CE2 | PHE A 128 | 21.325 | 67.993 | 23.183 | 1.00 | 10.05 | 6 ^{UN} |
| 993 | CE | LYS A 123 | 19.601 | 56.014 | 38.025 | 1.00 | 21.38 | 6 | 1035 | CZ | PHE A 128 | 21.229 | 67.218 | 22.070 | 1.00 | 10.20 | 6 |
| 994 | NZ | LYS A 123 | 20.133 | 55.054 | 39.000 | 1.00 | 25.83 | 7 | 1036 | N | VAL A 129 | 25.985 | 67.736 | 23.647 | 1.00 | 8.13 | 7 |
| 995 | N | VAL A 124 | 22.372 | 54.936 | 32.656 | 1.00 | 9.54 | 7 | 1037 | CA | VAL A 129 | 26.851 | 68.932 | 23.398 | 1.00 | 9.78 | 6 |
| 996 | CA | VAL A 124 | 23.343 | 55.533 | 31.740 | 1.00 | 9.53 | 6 | 1038 | C | VAL A 129 | 26.171 | 69.845 | 22.412 | 1.00 | 9.18 | 6 |
| 997 | C | VAL A 124 | 22.856 | 56.954 | 31.460 | 1.00 | 12.31 | 6 | 1039 | O | VAL A 129 | 26.494 | 70.026 | 21.210 | 1.00 | 10.74 | 8 |
| 998 | O | VAL A 124 | 21.723 | 57.168 | 30.990 | 1.00 | 12.23 | 8 | 1040 | CB | VAL A 129 | 28.178 | 68.381 | 22.804 | 1.00 | 11.28 | 6 |
| 999 | CB | VAL A 124 | 23.372 | 54.748 | 30.408 | 1.00 | 12.71 | 6 | 1041 | CG1 | VAL A 129 | 29.206 | 69.539 | 22.719 | 1.00 | 12.02 | 6 |
| 1000 | CG1 | VAL A 124 | 24.327 | 55.480 | 29.398 | 1.00 | 12.93 | 6 | 1042 | CG2 | VAL A 129 | 28.829 | 67.246 | 23.590 | 1.00 | 10.62 | 6 |
| 1001 | CG2 | VAL A 124 | 23.875 | 53.313 | 30.661 | 1.00 | 11.85 | 6 | 1043 | N | PRO A 130 | 25.165 | 70.638 | 22.855 | 1.00 | 10.64 | 6 |
| 1002 | N | ILE A 125 | 23.726 | 57.937 | 31.756 | 1.00 | 10.85 | 7 | 1044 | CA | PRO A 130 | 24.341 | 71.474 | 22.986 | 1.00 | 10.69 | 6 |
| 1003 | CA | ILE A 125 | 23.419 | 59.311 | 31.352 | 1.00 | 10.22 | 6 | 1045 | C | PRO A 130 | 24.946 | 72.802 | 21.588 | 1.00 | 11.36 | 6 |
| 1004 | C | ILE A 125 | 24.430 | 59.676 | 30.232 | 1.00 | 11.59 | 6 | 1046 | O | PRO A 130 | 24.336 | 73.565 | 20.814 | 1.00 | 11.49 | 8 |
| 1005 | O | ILE A 125 | 25.549 | 59.113 | 30.220 | 1.00 | 12.11 | 8 | 1047 | CB | PRO A 130 | 22.983 | 71.673 | 22.735 | 1.00 | 10.77 | 6 |
| 1006 | CB | ILE A 125 | 23.403 | 60.385 | 32.474 | 1.00 | 10.25 | 6 | 1048 | CG | PRO A 130 | 23.480 | 71.602 | 24.189 | 1.00 | 12.02 | 6 |
| 1007 | CG1 | ILE A 125 | 24.811 | 60.531 | 33.089 | 1.00 | 13.12 | 6 | 1049 | CD | PRO A 130 | 24.593 | 70.514 | 24.205 | 1.00 | 11.44 | 6 |
| 1008 | CG2 | ILE A 125 | 22.304 | 60.035 | 33.484 | 1.00 | 9.99 | 6 | 1050 | N | ASN A 131 | 26.107 | 73.181 | 22.144 | 1.00 | 9.48 | 7 |
| 1009 | CD1 | ILE A 125 | 24.770 | 61.746 | 34.084 | 1.00 | 17.03 | 6 | 1051 | CA | ASN A 131 | 26.687 | 74.481 | 21.859 | 1.00 | 10.43 | 6 |
| 1010 | N | VAL A 126 | 23.971 | 60.450 | 29.252 | 1.00 | 9.62 | 7 | 1052 | C | ASN A 131 | 27.244 | 74.637 | 20.438 | 1.00 | 11.66 | 6 |
| 1011 | CA | VAL A 126 | 24.864 | 60.725 | 28.102 | 1.00 | 10.33 | 6 | 1053 | O | ASN A 131 | 27.256 | 75.724 | 19.881 | 1.00 | 11.65 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1054 | CB | ASN A 131 | 27.756 | 74.902 | 22.877 | 1.00 | 10.94 | 6 | 1096 | CE1 | PHE A 136 | 33.813 | 78.477 | 13.738 | 1.00 | 13.44 | 6 |
| 1055 | CG | ASN A 131 | 28.233 | 76.316 | 22.592 | 1.00 | 10.72 | 6 | 1097 | CE2 | PHE A 136 | 34.451 | 79.741 | 11.779 | 1.00 | 12.17 | 6 |
| 1056 | OD1 | ASN A 131 | 27.396 | 77.205 | 22.783 | 1.00 | 10.02 | 8 | 1098 | CZ | PHE A 136 | 33.903 | 79.708 | 13.087 | 1.00 | 15.41 | 6 |
| 1057 | ND2 | ASN A 131 | 29.516 | 76.447 | 22.224 | 1.00 | 10.08 | 7 | 1099 | N | LYS A 137 | 38.037 | 77.258 | 10.547 | 1.00 | 11.70 | 7 |
| 1058 | N | HIS A 132 | 27.676 | 73.513 | 19.855 | 1.00 | 10.71 | 7 | 1100 | CA | LYS A 137 | 38.710 | 78.567 | 10.479 | 1.00 | 10.33 | 6 |
| 1059 | CA | HIS A 132 | 28.476 | 73.726 | 18.632 | 1.00 | 9.32 | 6 | 1101 | C | LYS A 137 | 37.859 | 79.484 | 9.618 | 1.00 | 13.10 | 6 |
| 1060 | C | HIS A 132 | 28.552 | 72.441 | 17.845 | 1.00 | 9.83 | 6 | 1102 | O | LYS A 137 | 37.493 | 79.111 | 8.490 | 1.00 | 12.91 | 8 |
| 1061 | O | HIS A 132 | 28.256 | 71.362 | 18.361 | 1.00 | 12.46 | 8 | 1103 | CB | LYS A 137 | 40.060 | 78.360 | 9.724 | 1.00 | 17.76 | 6 |
| 1062 | CB | HIS A 132 | 29.896 | 74.227 | 19.005 | 1.00 | 11.52 | 6 | 1104 | CG | LYS A 137 | 41.153 | 77.554 | 10.411 | 1.00 | 19.69 | 6 |
| 1063 | CG | HIS A 132 | 30.560 | 73.394 | 20.080 | 1.00 | 10.70 | 6 | 1105 | CD | LYS A 137 | 41.439 | 78.049 | 11.810 | 1.00 | 22.72 | 6 |
| 1064 | ND1 | HIS A 132 | 30.616 | 73.869 | 21.372 | 1.00 | 11.00 | 7 | 1106 | CE | LYS A 137 | 42.145 | 79.366 | 12.006 | 1.00 | 31.41 | 6 |
| 1065 | CD2 | HIS A 132 | 31.084 | 72.152 | 20.032 | 1.00 | 9.99 | 6 | 1107 | NZ | LYS A 137 | 43.212 | 79.771 | 11.035 | 1.00 | 25.39 | 7 |
| 1066 | CE1 | HIS A 132 | 31.189 | 72.945 | 22.154 | 1.00 | 12.39 | 6 | 1108 | N | ALA A 138 | 37.657 | 80.688 | 10.158 | 1.00 | 12.09 | 7 |
| 1067 | NE2 | HIS A 132 | 31.445 | 71.929 | 21.368 | 1.00 | 10.00 | 7 | 1109 | CA | ALA A 138 | 36.683 | 81.510 | 9.375 | 1.00 | 12.57 | 6 |
| 1068 | N | SER A 133 | 28.999 | 72.608 | 16.584 | 1.00 | 10.23 | 7 | 1110 | C | ALA A 138 | 37.267 | 81.873 | 8.017 | 1.00 | 14.60 | 6 |
| 1069 | CA | SER A 133 | 29.365 | 71.428 | 15.787 | 1.00 | 10.30 | 6 | 1111 | O | ALA A 138 | 36.469 | 82.176 | 7.094 | 1.00 | 14.01 | 8 |
| 1070 | C | SER A 133 | 30.876 | 71.239 | 15.861 | 1.00 | 11.64 | 6 | 1112 | CB | ALA A 138 | 36.410 | 82.806 | 10.148 | 1.00 | 15.45 | 6 |
| 1071 | O | SER A 133 | 31.319 | 70.652 | 16.863 | 1.00 | 11.94 | 8 | 1113 | N | ASN A 139 | 38.597 | 81.986 | 7.900 | 1.00 | 13.25 | 7 |
| 1072 | CB | SER A 133 | 28.807 | 71.514 | 14.344 | 1.00 | 10.65 | 6 | 1114 | CA | ASN A 139 | 39.165 | 82.359 | 6.608 | 1.00 | 14.41 | 6 |
| 1073 | OG | SER A 133 | 29.342 | 72.683 | 13.700 | 1.00 | 11.57 | 8 | 1115 | C | ASN A 139 | 39.444 | 81.212 | 5.682 | 1.00 | 14.25 | 6 |
| 1074 | N | THR A 134 | 31.611 | 71.535 | 14.805 | 1.00 | 11.30 | 7 | 1116 | O | ASN A 139 | 40.047 | 81.349 | 4.562 | 1.00 | 14.82 | 8 |
| 1075 | CA | THR A 134 | 33.034 | 71.082 | 14.740 | 1.00 | 10.51 | 6 | 1117 | CB | ASN A 139 | 40.443 | 83.188 | 6.852 | 1.00 | 16.78 | 6 |
| 1076 | C | THR A 134 | 33.959 | 72.251 | 14.424 | 1.00 | 8.56 | 6 | 1118 | CG | ASN A 139 | 41.666 | 82.292 | 7.083 | 1.00 | 22.27 | 6 |
| 1077 | O | THR A 134 | 33.553 | 73.376 | 14.121 | 1.00 | 10.40 | 8 | 1119 | OD1 | ASN A 139 | 41.484 | 81.167 | 7.486 | 1.00 | 25.66 | 8 |
| 1078 | CB | THR A 134 | 33.119 | 70.005 | 13.630 | 1.00 | 9.65 | 6 | 1120 | ND2 | ASN A 139 | 42.853 | 82.762 | 6.773 | 1.00 | 21.53 | 7 |
| 1079 | OG1 | THR A 134 | 32.559 | 70.596 | 12.429 | 1.00 | 11.51 | 8 | 1121 | N | ASP A 140 | 39.150 | 79.955 | 6.052 | 1.00 | 14.76 | 7 |
| 1080 | CG2 | THR A 134 | 32.295 | 68.752 | 13.956 | 1.00 | 11.00 | 6 | 1122 | CA | ASP A 140 | 39.433 | 78.835 | 5.203 | 1.00 | 13.60 | 6 |
| 1081 | N | PRO A 135 | 35.256 | 71.959 | 14.489 | 1.00 | 10.51 | 7 | 1123 | C | ASP A 140 | 38.470 | 77.674 | 5.337 | 1.00 | 16.09 | 6 |
| 1082 | CA | PRO A 135 | 36.320 | 72.955 | 14.289 | 1.00 | 12.33 | 6 | 1124 | O | ASP A 140 | 38.607 | 76.905 | 6.339 | 1.00 | 13.95 | 8 |
| 1083 | C | PRO A 135 | 36.264 | 73.606 | 12.899 | 1.00 | 12.27 | 6 | 1125 | CB | ASP A 140 | 40.885 | 78.382 | 5.557 | 1.00 | 12.14 | 6 |
| 1084 | O | PRO A 135 | 36.014 | 72.968 | 11.868 | 1.00 | 13.19 | 8 | 1126 | CG | ASP A 140 | 41.331 | 77.260 | 4.643 | 1.00 | 16.87 | 6 |
| 1085 | CB | PRO A 135 | 37.627 | 72.145 | 14.405 | 1.00 | 11.11 | 6 | 1127 | OD1 | ASP A 140 | 40.616 | 76.705 | 3.810 | 1.00 | 17.82 | 8 |
| 1086 | CG | PRO A 135 | 37.241 | 71.129 | 15.486 | 1.00 | 11.56 | 6 | 1128 | OD2 | ASP A 140 | 42.569 | 76.954 | 4.814 | 1.00 | 25.09 | 8 |
| 1087 | CD | PRO A 135 | 35.809 | 70.746 | 15.111 | 1.00 | 11.98 | 6 | 1129 | N | SER A 141 | 37.529 | 77.555 | 4.414 | 1.00 | 15.21 | 7 |
| 1088 | N | PHE A 136 | 36.500 | 74.966 | 12.885 | 1.00 | 10.88 | 7 | 1130 | CA | SER A 141 | 36.508 | 76.520 | 4.501 | 1.00 | 16.63 | 6 |
| 1089 | CA | PHE A 136 | 36.606 | 75.628 | 11.597 | 1.00 | 11.37 | 6 | 1131 | C | SER A 141 | 37.048 | 75.092 | 4.285 | 1.00 | 17.44 | 6 |
| 1090 | O | PHE A 136 | 37.536 | 76.830 | 11.718 | 1.00 | 11.99 | 6 | 1132 | O | SER A 141 | 36.349 | 74.129 | 4.607 | 1.00 | 18.28 | 8 |
| 1091 | C | PHE A 136 | 37.856 | 77.248 | 12.827 | 1.00 | 12.95 | 8 | 1133 | CB | SER A 141 | 35.372 | 76.746 | 3.493 | 1.00 | 19.52 | 6 |
| 1092 | CB | PHE A 136 | 35.176 | 76.074 | 11.125 | 1.00 | 13.36 | 6 | 1134 | OG | SER A 141 | 35.867 | 76.579 | 2.144 | 1.00 | 16.38 | 8 |
| 1093 | CG | PHE A 136 | 34.690 | 77.341 | 11.793 | 1.00 | 15.31 | 6 | 1135 | N | THR A 142 | 38.302 | 74.958 | 3.839 | 1.00 | 14.08 | 7 |
| 1094 | CD1 | PHE A 136 | 34.201 | 77.311 | 13.100 | 1.00 | 12.18 | 6 | 1136 | CA | THR A 142 | 38.889 | 73.615 | 3.649 | 1.00 | 15.63 | 6 |
| 1095 | CD2 | PHE A 136 | 34.801 | 78.565 | 11.134 | 1.00 | 13.24 | 6 | 1137 | C | THR A 142 | 39.445 | 73.036 | 4.933 | 1.00 | 16.91 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1138 | O | THR A 142 | 39.798 | 71.840 | 4.961 | 1.00 | 15.67 | 8 | 1180 | N | LEU A 149 | 27.188 | 70.305 | 9.543 | 1.00 | 12.19 | 7 |
| 1139 | CB | THR A 142 | 40.105 | 73.658 | 2.622 | 1.00 | 16.59 | 6 | 1181 | CA | LEU A 149 | 26.192 | 69.594 | 10.365 | 1.00 | 10.39 | 6 |
| 1140 | OG1 | THR A 142 | 41.261 | 74.288 | 3.211 | 1.00 | 18.35 | 8 | 1182 | C | LEU A 149 | 25.298 | 68.798 | 9.407 | 1.00 | 10.91 | 6 |
| 1141 | CG2 | THR A 142 | 39.653 | 74.352 | 1.368 | 1.00 | 25.03 | 6 | 1183 | O | LEU A 149 | 24.907 | 69.311 | 8.313 | 1.00 | 14.52 | 8 |
| 1142 | N | PHE A 143 | 39.533 | 73.874 | 6.007 | 1.00 | 15.48 | 7 | 1184 | CB | LEU A 149 | 25.345 | 70.684 | 11.028 | 1.00 | 10.56 | 6 |
| 1143 | CA | PHE A 143 | 40.027 | 73.314 | 7.285 | 1.00 | 12.99 | 6 | 1185 | CG | LEU A 149 | 24.344 | 70.222 | 12.098 | 1.00 | 14.34 | 6 |
| 1144 | C | PHE A 143 | 38.953 | 72.384 | 7.908 | 1.00 | 14.57 | 6 | 1186 | CD1 | LEU A 149 | 25.067 | 69.618 | 13.294 | 1.00 | 16.21 | 6 |
| 1145 | O | PHE A 143 | 37.807 | 72.837 | 8.026 | 1.00 | 12.49 | 8 | 1187 | CD2 | LEU A 149 | 23.436 | 71.409 | 12.447 | 1.00 | 15.60 | 6 |
| 1146 | CB | PHE A 143 | 40.412 | 74.481 | 8.238 | 1.00 | 14.72 | 6 | 1188 | N | TYR A 150 | 25.047 | 67.560 | 9.836 | 1.00 | 12.69 | 7 |
| 1147 | CG | PHE A 143 | 40.905 | 73.939 | 9.546 | 1.00 | 13.33 | 6 | 1189 | CA | TYR A 150 | 24.178 | 66.675 | 9.057 | 1.00 | 11.91 | 6 |
| 1148 | CD1 | PHE A 143 | 42.192 | 73.454 | 9.669 | 1.00 | 14.66 | 6 | 1190 | C | TYR A 150 | 23.007 | 66.234 | 9.957 | 1.00 | 13.54 | 6 |
| 1149 | CD2 | PHE A 143 | 40.054 | 73.908 | 10.679 | 1.00 | 10.60 | 6 | 1191 | O | TYR A 150 | 23.116 | 66.203 | 11.188 | 1.00 | 12.53 | 8 |
| 1150 | CE1 | PHE A 143 | 42.677 | 72.946 | 10.878 | 1.00 | 14.87 | 6 | 1192 | CB | TYR A 150 | 24.945 | 65.392 | 8.671 | 1.00 | 12.62 | 6 |
| 1151 | CE2 | PHE A 143 | 40.556 | 73.381 | 11.849 | 1.00 | 12.09 | 6 | 1193 | CG | TYR A 150 | 26.104 | 65.699 | 7.694 | 1.00 | 10.80 | 6 |
| 1152 | CZ | PHE A 143 | 41.842 | 72.912 | 11.975 | 1.00 | 16.30 | 6 | 1194 | CD1 | TYR A 150 | 27.275 | 66.240 | 8.185 | 1.00 | 13.28 | 6 |
| 1153 | N | ALA A 144 | 39.342 | 71.174 | 8.264 | 1.00 | 14.83 | 7 | 1195 | CD2 | TYR A 150 | 25.983 | 65.330 | 6.359 | 1.00 | 14.10 | 6 |
| 1154 | CA | ALA A 144 | 38.380 | 70.250 | 8.884 | 1.00 | 14.49 | 6 | 1196 | CE1 | TYR A 150 | 28.295 | 66.545 | 7.273 | 1.00 | 14.81 | 6 |
| 1155 | C | ALA A 144 | 37.165 | 70.136 | 7.976 | 1.00 | 10.16 | 6 | 1197 | CE2 | TYR A 150 | 27.004 | 65.609 | 5.479 | 1.00 | 17.28 | 6 |
| 1156 | O | ALA A 144 | 37.369 | 69.878 | 6.784 | 1.00 | 13.97 | 8 | 1198 | CZ | TYR A 150 | 28.139 | 66.206 | 5.959 | 1.00 | 17.89 | 6 |
| 1157 | CB | ALA A 144 | 37.990 | 70.683 | 10.323 | 1.00 | 12.28 | 6 | 1199 | OH | TYR A 150 | 29.227 | 66.444 | 5.082 | 1.00 | 18.31 | 8 |
| 1158 | N | GLU A 145 | 35.942 | 70.135 | 8.506 | 1.00 | 11.43 | 7 | 1200 | N | ASN A 151 | 21.932 | 65.787 | 9.288 | 1.00 | 11.59 | 7 |
| 1159 | CA | GLU A 145 | 34.744 | 70.061 | 7.645 | 1.00 | 10.19 | 6 | 1201 | CA | ASN A 151 | 20.774 | 65.261 | 10.048 | 1.00 | 13.13 | 6 |
| 1160 | C | GLU A 145 | 34.063 | 71.386 | 7.520 | 1.00 | 10.66 | 6 | 1202 | C | ASN A 151 | 20.582 | 63.801 | 9.659 | 1.00 | 14.46 | 6 |
| 1161 | O | GLU A 145 | 32.824 | 71.513 | 7.266 | 1.00 | 11.84 | 8 | 1203 | O | ASN A 151 | 20.020 | 63.527 | 8.595 | 1.00 | 15.41 | 8 |
| 1162 | CB | GLU A 145 | 33.771 | 68.943 | 8.180 | 1.00 | 11.91 | 6 | 1204 | CB | ASN A 151 | 19.542 | 66.068 | 9.633 | 1.00 | 12.78 | 6 |
| 1163 | CG | GLU A 145 | 34.408 | 67.577 | 8.042 | 1.00 | 11.68 | 6 | 1205 | CG | ASN A 151 | 18.280 | 65.607 | 10.386 | 1.00 | 15.85 | 6 |
| 1164 | CD | GLU A 145 | 33.591 | 66.467 | 8.697 | 1.00 | 15.77 | 6 | 1206 | OD1 | ASN A 151 | 18.376 | 65.084 | 11.460 | 1.00 | 14.91 | 8 |
| 1165 | OE1 | GLU A 145 | 32.530 | 66.660 | 9.208 | 1.00 | 20.95 | 8 | 1207 | ND2 | ASN A 151 | 17.115 | 65.851 | 9.790 | 1.00 | 23.13 | 7 |
| 1166 | OE2 | GLU A 145 | 34.122 | 65.351 | 8.743 | 1.00 | 21.22 | 8 | 1208 | N | ASN A 152 | 21.153 | 62.881 | 10.455 | 1.00 | 11.88 | 7 |
| 1167 | N | GLY A 146 | 34.677 | 72.533 | 7.898 | 1.00 | 12.55 | 7 | 1209 | CA | ASN A 152 | 21.160 | 61.460 | 10.056 | 1.00 | 12.91 | 6 |
| 1168 | CA | GLY A 146 | 34.021 | 73.826 | 7.783 | 1.00 | 12.03 | 6 | 1210 | C | ASN A 152 | 21.628 | 61.265 | 8.619 | 1.00 | 17.10 | 6 |
| 1169 | C | GLY A 146 | 32.799 | 73.976 | 8.739 | 1.00 | 15.18 | 6 | 1211 | O | ASN A 152 | 21.059 | 60.495 | 7.804 | 1.00 | 18.15 | 8 |
| 1170 | O | GLY A 146 | 32.025 | 74.880 | 8.511 | 1.00 | 13.95 | 8 | 1212 | CB | ASN A 152 | 19.763 | 60.894 | 10.305 | 1.00 | 15.18 | 6 |
| 1171 | N | GLY A 147 | 32.774 | 73.157 | 9.790 | 1.00 | 12.57 | 7 | 1213 | CG | ASN A 152 | 19.772 | 59.363 | 10.289 | 1.00 | 28.25 | 6 |
| 1172 | CA | GLY A 147 | 31.639 | 73.265 | 10.703 | 1.00 | 12.28 | 6 | 1214 | OD1 | ASN A 152 | 20.803 | 58.741 | 10.579 | 1.00 | 25.62 | 8 |
| 1173 | C | GLY A 147 | 30.439 | 72.415 | 10.267 | 1.00 | 14.09 | 6 | 1215 | ND2 | ASN A 152 | 18.647 | 58.722 | 9.925 | 1.00 | 26.09 | 7 |
| 1174 | O | GLY A 147 | 29.372 | 72.644 | 10.903 | 1.00 | 11.87 | 8 | 1216 | N | GLY A 153 | 22.797 | 61.857 | 8.344 | 1.00 | 11.86 | 7 |
| 1175 | N | ALA A 148 | 30.552 | 71.583 | 9.258 | 1.00 | 11.40 | 7 | 1217 | CA | GLY A 153 | 23.494 | 61.698 | 7.061 | 1.00 | 15.63 | 6 |
| 1176 | CA | ALA A 148 | 29.343 | 70.942 | 8.707 | 1.00 | 13.48 | 6 | 1218 | C | GLY A 153 | 23.096 | 62.727 | 6.007 | 1.00 | 17.70 | 6 |
| 1177 | C | ALA A 148 | 28.495 | 70.132 | 9.729 | 1.00 | 11.58 | 6 | 1219 | O | GLY A 153 | 23.819 | 62.836 | 4.994 | 1.00 | 16.41 | 8 |
| 1178 | O | ALA A 148 | 29.025 | 69.390 | 10.557 | 1.00 | 12.14 | 8 | 1220 | N | THR A 154 | 21.975 | 63.414 | 6.209 | 1.00 | 13.77 | 7 |
| 1179 | CB | ALA A 148 | 29.861 | 69.927 | 7.660 | 1.00 | 14.52 | 6 | 1221 | CA | THR A 154 | 21.535 | 64.406 | 5.220 | 1.00 | 14.28 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1222 | C | THR A 154 | 22.181 | 65.781 | 5.538 | 1.00 | 14.24 | 6 | 1264 | CG | TYR A 159 | 31.171 | 79.475 | 10.063 | 1.00 | 11.61 | 6 |
| 1223 | O | THR A 154 | 22.048 | 66.264 | 6.650 | 1.00 | 15.31 | 8 | 1265 | CD1 | TYR A 159 | 30.414 | 79.868 | 11.149 | 1.00 | 14.86 | 6 |
| 1224 | CB | THR A 154 | 20.008 | 64.592 | 5.212 | 1.00 | 21.10 | 6 | 1266 | CD2 | TYR A 159 | 31.962 | 80.402 | 9.380 | 1.00 | 13.87 | 6 |
| 1225 | OG1 | THR A 154 | 19.488 | 63.334 | 4.709 | 1.00 | 20.66 | 8 | 1267 | CE1 | TYR A 159 | 30.576 | 81.181 | 11.600 | 1.00 | 15.19 | 6 |
| 1226 | CG2 | THR A 154 | 19.569 | 65.711 | 4.260 | 1.00 | 21.99 | 6 | 1268 | CE2 | TYR A 159 | 32.069 | 81.716 | 9.811 | 1.00 | 19.88 | 6 |
| 1227 | N | TYR A 155 | 22.977 | 66.280 | 4.566 | 1.00 | 14.57 | 7 | 1269 | CZ | TYR A 159 | 31.387 | 82.088 | 10.926 | 1.00 | 16.15 | 6 |
| 1228 | CA | TYR A 155 | 23.613 | 67.573 | 4.928 | 1.00 | 15.65 | 6 | 1270 | OH | TYR A 159 | 31.377 | 83.383 | 11.432 | 1.00 | 16.24 | 8 |
| 1229 | C | TYR A 155 | 22.652 | 68.698 | 5.184 | 1.00 | 17.55 | 6 | 1271 | N | PHE A 160 | 29.904 | 78.307 | 6.253 | 1.00 | 13.52 | 7 |
| 1230 | O | TYR A 155 | 21.639 | 68.912 | 4.487 | 1.00 | 16.44 | 8 | 1272 | CA | PHE A 160 | 30.073 | 79.126 | 5.029 | 1.00 | 12.84 | 6 |
| 1231 | CB | TYR A 155 | 24.440 | 67.984 | 3.678 | 1.00 | 16.08 | 6 | 1273 | C | PHE A 160 | 28.855 | 79.182 | 4.153 | 1.00 | 12.34 | 6 |
| 1232 | CG | TYR A 155 | 25.238 | 69.243 | 3.820 | 1.00 | 16.71 | 6 | 1274 | O | PHE A 160 | 28.803 | 80.101 | 3.300 | 1.00 | 14.63 | 8 |
| 1233 | CD1 | TYR A 155 | 26.324 | 69.277 | 4.693 | 1.00 | 16.20 | 6 | 1275 | CB | PHE A 160 | 31.228 | 78.421 | 4.234 | 1.00 | 12.99 | 6 |
| 1234 | CD2 | TYR A 155 | 24.989 | 70.381 | 3.075 | 1.00 | 16.54 | 6 | 1276 | CG | PHE A 160 | 32.504 | 78.508 | 5.080 | 1.00 | 14.21 | 6 |
| 1235 | CE1 | TYR A 155 | 27.139 | 70.407 | 4.789 | 1.00 | 16.44 | 6 | 1277 | CD1 | PHE A 160 | 33.310 | 79.562 | 4.935 | 1.00 | 12.64 | 6 |
| 1236 | CE2 | TYR A 155 | 25.773 | 71.530 | 3.162 | 1.00 | 14.17 | 6 | 1278 | CD2 | PHE A 160 | 32.804 | 77.488 | 5.965 | 1.00 | 12.84 | 6 |
| 1237 | CZ | TYR A 155 | 26.843 | 71.515 | 4.015 | 1.00 | 16.83 | 6 | 1279 | CE1 | PHE A 160 | 34.466 | 79.772 | 5.737 | 1.00 | 14.91 | 6 |
| 1238 | OH | TYR A 155 | 27.673 | 72.601 | 4.142 | 1.00 | 15.80 | 8 | 1280 | CE2 | PHE A 160 | 33.940 | 77.621 | 6.761 | 1.00 | 14.27 | 6 |
| 1239 | N | MET A 156 | 22.895 | 69.456 | 6.272 | 1.00 | 12.36 | 7 | 1281 | CZ | PHE A 160 | 34.769 | 78.740 | 6.553 | 1.00 | 13.93 | 6 |
| 1240 | CA | MET A 156 | 22.120 | 70.658 | 6.595 | 1.00 | 12.72 | 6 | 1282 | N | ASP A 161 | 27.917 | 78.220 | 4.232 | 1.00 | 14.16 | 7 |
| 1241 | C | MET A 156 | 22.877 | 71.939 | 6.202 | 1.00 | 14.70 | 6 | 1283 | CA | ASP A 161 | 26.731 | 78.329 | 3.371 | 1.00 | 14.46 | 6 |
| 1242 | O | MET A 156 | 22.290 | 72.876 | 5.628 | 1.00 | 14.86 | 8 | 1284 | C | ASP A 161 | 25.486 | 78.622 | 4.217 | 1.00 | 14.25 | 6 |
| 1243 | CB | MET A 156 | 21.886 | 70.683 | 8.141 | 1.00 | 14.72 | 6 | 1285 | O | ASP A 161 | 24.375 | 78.215 | 3.808 | 1.00 | 15.23 | 8 |
| 1244 | CG | MET A 156 | 21.045 | 69.510 | 8.543 | 1.00 | 13.16 | 6 | 1286 | CB | ASP A 161 | 26.557 | 77.031 | 2.565 | 1.00 | 12.66 | 6 |
| 1245 | SD | MET A 156 | 20.812 | 69.391 | 10.354 | 1.00 | 16.44 | 16 | 1287 | CG | ASP A 161 | 26.500 | 75.766 | 3.373 | 1.00 | 15.72 | 6 |
| 1246 | CE | MET A 156 | 19.828 | 70.788 | 10.735 | 1.00 | 16.14 | 6 | 1288 | OD1 | ASP A 161 | 26.191 | 75.896 | 4.579 | 1.00 | 13.04 | 8 |
| 1247 | N | GLY A 157 | 24.138 | 72.003 | 6.634 | 1.00 | 15.28 | 7 | 1289 | OD2 | ASP A 161 | 26.767 | 74.716 | 2.766 | 1.00 | 20.26 | 8 |
| 1248 | CA | GLY A 157 | 24.888 | 73.257 | 6.260 | 1.00 | 12.22 | 6 | 1290 | N | ASP A 162 | 25.656 | 79.460 | 5.227 | 1.00 | 13.84 | 7 |
| 1249 | C | GLY A 157 | 26.169 | 73.337 | 7.061 | 1.00 | 15.29 | 6 | 1291 | CA | ASP A 162 | 24.557 | 79.667 | 6.196 | 1.00 | 14.60 | 6 |
| 1250 | O | GLY A 157 | 26.402 | 72.513 | 7.965 | 1.00 | 13.96 | 8 | 1292 | C | ASP A 162 | 23.787 | 80.939 | 5.979 | 1.00 | 16.54 | 6 |
| 1251 | N | ASN A 158 | 26.981 | 74.369 | 6.736 | 1.00 | 13.19 | 7 | 1293 | O | ASP A 162 | 22.840 | 81.252 | 6.726 | 1.00 | 18.25 | 8 |
| 1252 | CA | ASN A 158 | 28.205 | 74.586 | 7.495 | 1.00 | 12.06 | 6 | 1294 | CB | ASP A 162 | 25.253 | 79.785 | 7.584 | 1.00 | 12.11 | 6 |
| 1253 | C | ASN A 158 | 28.353 | 76.085 | 7.759 | 1.00 | 8.80 | 6 | 1295 | CG | ASP A 162 | 24.264 | 79.524 | 8.717 | 1.00 | 13.12 | 6 |
| 1254 | O | ASN A 158 | 27.377 | 76.850 | 7.583 | 1.00 | 11.73 | 8 | 1296 | OD1 | ASP A 162 | 23.408 | 78.624 | 8.551 | 1.00 | 12.76 | 8 |
| 1255 | CB | ASN A 158 | 29.438 | 73.957 | 6.787 | 1.00 | 12.79 | 6 | 1297 | OD2 | ASP A 162 | 24.417 | 80.201 | 9.775 | 1.00 | 12.76 | 8 |
| 1256 | CG | ASN A 158 | 29.783 | 74.647 | 5.457 | 1.00 | 16.08 | 6 | 1298 | N | ALA A 163 | 24.109 | 81.725 | 4.949 | 1.00 | 16.09 | 7 |
| 1257 | OD1 | ASN A 158 | 29.311 | 75.727 | 5.160 | 1.00 | 12.69 | 8 | 1299 | CA | ALA A 163 | 23.428 | 83.019 | 4.792 | 1.00 | 16.11 | 6 |
| 1258 | ND2 | ASN A 158 | 30.650 | 74.060 | 4.603 | 1.00 | 20.88 | 7 | 1300 | C | ALA A 163 | 21.914 | 82.901 | 4.848 | 1.00 | 17.25 | 6 |
| 1259 | N | TYR A 159 | 29.559 | 76.484 | 8.260 | 1.00 | 10.67 | 7 | 1301 | O | ALA A 163 | 21.341 | 83.825 | 5.467 | 1.00 | 24.30 | 8 |
| 1260 | CA | TYR A 159 | 29.714 | 77.924 | 8.640 | 1.00 | 11.67 | 6 | 1302 | CB | ALA A 163 | 23.828 | 83.609 | 3.414 | 1.00 | 19.57 | 6 |
| 1261 | C | TYR A 159 | 29.665 | 78.827 | 7.432 | 1.00 | 12.87 | 6 | 1303 | N | THR A 164 | 21.317 | 81.987 | 4.145 | 1.00 | 19.25 | 7 |
| 1262 | O | TYR A 159 | 29.444 | 80.029 | 7.605 | 1.00 | 12.70 | 8 | 1304 | CA | THR A 164 | 19.845 | 81.973 | 4.121 | 1.00 | 24.11 | 6 |
| 1263 | CB | TYR A 159 | 31.055 | 78.072 | 9.434 | 1.00 | 11.86 | 6 | 1305 | C | THR A 164 | 19.237 | 81.014 | 5.149 | 1.00 | 25.86 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1306 | O | THR A 164 | 18.055 | 80.605 | 5.002 | 1.00 | 25.38 | 8 | 1348 | C | HIS A 169 | 27.266 | 82.836 | 14.195 | 1.00 | 11.69 | 6 |
| 1307 | CB | THR A 164 | 19.384 | 81.502 | 2.723 | 1.00 | 21.33 | 6 | 1349 | O | HIS A 169 | 28.109 | 82.035 | 13.921 | 1.00 | 11.66 | 8 |
| 1308 | OG1 | THR A 164 | 19.834 | 80.146 | 2.496 | 1.00 | 29.22 | 8 | 1350 | CB | HIS A 169 | 26.361 | 82.658 | 16.482 | 1.00 | 11.57 | 6 |
| 1309 | CG2 | THR A 164 | 20.062 | 82.359 | 1.658 | 1.00 | 32.67 | 6 | 1351 | CG | HIS A 169 | 25.157 | 82.347 | 17.376 | 1.00 | 11.97 | 6 |
| 1310 | N | LYS A 165 | 20.086 | 80.431 | 6.008 | 1.00 | 19.16 | 7 | 1352 | ND1 | HIS A 169 | 25.403 | 81.657 | 18.588 | 1.00 | 11.36 | 7 |
| 1311 | CA | LYS A 165 | 19.577 | 79.430 | 6.929 | 1.00 | 16.62 | 6 | 1353 | CD2 | HIS A 169 | 23.838 | 82.604 | 17.274 | 1.00 | 11.55 | 6 |
| 1312 | C | LYS A 165 | 19.714 | 79.888 | 8.391 | 1.00 | 18.03 | 6 | 1354 | CE1 | HIS A 169 | 24.195 | 81.518 | 19.195 | 1.00 | 12.02 | 6 |
| 1313 | O | LYS A 165 | 18.735 | 79.767 | 9.173 | 1.00 | 17.25 | 8 | 1355 | NE2 | HIS A 169 | 23.233 | 82.111 | 18.427 | 1.00 | 10.80 | 7 |
| 1314 | CB | LYS A 165 | 20.423 | 78.140 | 6.826 | 1.00 | 13.80 | 6 | 1356 | N | HIS A 170 | 27.295 | 84.147 | 13.797 | 1.00 | 11.77 | 7 |
| 1315 | CG | LYS A 165 | 20.215 | 77.497 | 5.423 | 1.00 | 21.49 | 6 | 1357 | CA | HIS A 170 | 28.474 | 84.629 | 13.015 | 1.00 | 12.20 | 6 |
| 1316 | CD | LYS A 165 | 20.913 | 76.186 | 5.334 | 1.00 | 30.47 | 6 | 1358 | C | HIS A 170 | 29.029 | 85.872 | 13.672 | 1.00 | 14.93 | 6 |
| 1317 | CE | LYS A 165 | 22.394 | 76.297 | 5.245 | 1.00 | 26.09 | 6 | 1359 | O | HIS A 170 | 29.174 | 86.974 | 13.053 | 1.00 | 16.92 | 8 |
| 1318 | NZ | LYS A 165 | 23.067 | 75.308 | 4.349 | 1.00 | 18.44 | 7 | 1360 | CB | HIS A 170 | 28.083 | 84.949 | 11.533 | 1.00 | 13.28 | 6 |
| 1319 | N | GLY A 166 | 20.839 | 80.499 | 8.700 | 1.00 | 14.27 | 7 | 1361 | CG | HIS A 170 | 27.535 | 83.698 | 10.888 | 1.00 | 12.02 | 6 |
| 1320 | CA | GLY A 166 | 21.048 | 81.024 | 10.082 | 1.00 | 14.43 | 6 | 1362 | ND1 | HIS A 170 | 28.327 | 82.925 | 10.069 | 1.00 | 15.51 | 7 |
| 1321 | C | GLY A 166 | 21.103 | 79.863 | 11.109 | 1.00 | 14.80 | 6 | 1363 | CD2 | HIS A 170 | 26.306 | 83.088 | 10.915 | 1.00 | 13.12 | 6 |
| 1322 | O | GLY A 166 | 20.730 | 80.096 | 12.287 | 1.00 | 14.92 | 8 | 1364 | CE1 | HIS A 170 | 27.639 | 81.863 | 9.689 | 1.00 | 16.69 | 6 |
| 1323 | N | TYR A 167 | 21.732 | 78.765 | 10.734 | 1.00 | 12.78 | 7 | 1365 | NE2 | HIS A 170 | 26.409 | 81.953 | 10.156 | 1.00 | 13.32 | 7 |
| 1324 | CA | TYR A 167 | 21.882 | 77.692 | 11.732 | 1.00 | 12.54 | 6 | 1366 | N | ASN A 171 | 29.387 | 85.778 | 14.962 | 1.00 | 12.58 | 7 |
| 1325 | C | TYR A 167 | 22.991 | 78.009 | 12.739 | 1.00 | 12.62 | 6 | 1367 | CA | ASN A 171 | 29.735 | 86.967 | 15.733 | 1.00 | 12.76 | 6 |
| 1326 | O | TYR A 167 | 23.085 | 77.349 | 13.776 | 1.00 | 11.78 | 8 | 1368 | C | ASN A 171 | 31.201 | 87.040 | 16.147 | 1.00 | 13.34 | 6 |
| 1327 | CB | TYR A 167 | 22.226 | 76.374 | 11.022 | 1.00 | 10.92 | 6 | 1369 | O | ASN A 171 | 31.554 | 87.947 | 16.949 | 1.00 | 17.31 | 8 |
| 1328 | CG | TYR A 167 | 21.127 | 75.836 | 10.103 | 1.00 | 14.63 | 6 | 1370 | CB | ASN A 171 | 28.916 | 86.961 | 17.054 | 1.00 | 13.40 | 6 |
| 1329 | CD1 | TYR A 167 | 19.810 | 76.232 | 10.291 | 1.00 | 13.59 | 6 | 1371 | CG | ASN A 171 | 27.430 | 86.948 | 16.719 | 1.00 | 17.12 | 6 |
| 1330 | CD2 | TYR A 167 | 21.490 | 74.921 | 9.121 | 1.00 | 15.06 | 6 | 1372 | OD1 | ASN A 171 | 26.595 | 86.168 | 17.252 | 1.00 | 16.54 | 8 |
| 1331 | CE1 | TYR A 167 | 18.836 | 75.722 | 9.421 | 1.00 | 13.53 | 6 | 1373 | ND2 | ASN A 171 | 27.046 | 87.866 | 15.861 | 1.00 | 12.82 | 7 |
| 1332 | CE2 | TYR A 167 | 20.503 | 74.385 | 8.254 | 1.00 | 12.93 | 6 | 1374 | N | GLY A 172 | 32.013 | 86.197 | 15.601 | 1.00 | 13.14 | 7 |
| 1333 | CZ | TYR A 167 | 19.211 | 74.809 | 8.469 | 1.00 | 15.10 | 6 | 1375 | CA | GLY A 172 | 33.444 | 86.166 | 15.964 | 1.00 | 15.42 | 6 |
| 1334 | OH | TYR A 167 | 18.235 | 74.289 | 7.594 | 1.00 | 18.52 | 8 | 1376 | C | GLY A 172 | 33.728 | 85.275 | 17.210 | 1.00 | 16.69 | 6 |
| 1335 | N | PHE A 168 | 23.963 | 78.870 | 12.342 | 1.00 | 11.36 | 7 | 1377 | O | GLY A 172 | 32.817 | 84.706 | 17.722 | 1.00 | 14.98 | 8 |
| 1336 | CA | PHE A 168 | 25.072 | 79.208 | 13.244 | 1.00 | 11.20 | 6 | 1378 | N | ASP A 173 | 34.993 | 85.180 | 17.526 | 1.00 | 14.76 | 7 |
| 1337 | C | PHE A 168 | 25.097 | 80.677 | 13.551 | 1.00 | 12.02 | 6 | 1379 | CA | ASP A 173 | 35.473 | 84.346 | 18.622 | 1.00 | 12.93 | 6 |
| 1338 | O | PHE A 168 | 24.515 | 81.539 | 12.854 | 1.00 | 11.21 | 8 | 1380 | C | ASP A 173 | 35.292 | 84.996 | 19.976 | 1.00 | 12.76 | 6 |
| 1339 | CB | PHE A 168 | 26.432 | 78.934 | 12.493 | 1.00 | 13.41 | 6 | 1381 | O | ASP A 173 | 35.410 | 86.248 | 20.131 | 1.00 | 11.79 | 8 |
| 1340 | CG | PHE A 168 | 26.552 | 77.459 | 12.174 | 1.00 | 11.52 | 6 | 1382 | CB | ASP A 173 | 36.980 | 84.152 | 18.369 | 1.00 | 14.28 | 6 |
| 1341 | CD1 | PHE A 168 | 27.044 | 76.583 | 13.130 | 1.00 | 10.63 | 6 | 1383 | CG | ASP A 173 | 37.273 | 83.139 | 17.268 | 1.00 | 24.98 | 6 |
| 1342 | CD2 | PHE A 168 | 26.171 | 77.007 | 10.899 | 1.00 | 13.81 | 6 | 1384 | OD1 | ASP A 173 | 36.398 | 82.387 | 16.822 | 1.00 | 17.11 | 8 |
| 1343 | CE1 | PHE A 168 | 27.122 | 75.214 | 12.765 | 1.00 | 12.04 | 6 | 1385 | OD2 | ASP A 173 | 38.451 | 83.124 | 16.815 | 1.00 | 23.71 | 8 |
| 1344 | CE2 | PHE A 168 | 26.250 | 75.639 | 10.574 | 1.00 | 12.05 | 6 | 1386 | N | ILE A 174 | 35.073 | 84.127 | 20.969 | 1.00 | 12.58 | 7 |
| 1345 | CZ | PHE A 168 | 26.752 | 74.751 | 11.518 | 1.00 | 12.13 | 6 | 1387 | CA | ILE A 174 | 35.136 | 84.670 | 22.362 | 1.00 | 11.65 | 6 |
| 1346 | N | HIS A 169 | 25.665 | 81.067 | 14.709 | 1.00 | 11.43 | 7 | 1388 | C | ILE A 174 | 36.500 | 85.307 | 22.646 | 1.00 | 14.87 | 6 |
| 1347 | CA | HIS A 169 | 25.979 | 82.473 | 14.979 | 1.00 | 12.52 | 6 | 1389 | O | ILE A 174 | 37.508 | 84.670 | 22.337 | 1.00 | 15.09 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1390 | CB | ILE A 174 | 34.896 | 83.495 | 23.357 | 1.00 | 13.27 | 6 | 1432 | C | ASP A 179 | 30.292 | 87.603 | 28.903 | 1.00 | 12.33 | 6 |
| 1391 | CG1 | ILE A 174 | 33.431 | 83.005 | 23.177 | 1.00 | 10.95 | 6 | 1433 | O | ASP A 179 | 30.537 | 86.725 | 28.067 | 1.00 | 12.08 | 8 |
| 1392 | CG2 | ILE A 174 | 35.145 | 84.016 | 24.806 | 1.00 | 12.74 | 6 | 1434 | CB | ASP A 179 | 31.997 | 89.341 | 28.184 | 1.00 | 15.43 | 6 |
| 1393 | CD1 | ILE A 174 | 33.220 | 81.690 | 24.000 | 1.00 | 11.77 | 6 | 1435 | CG | ASP A 179 | 30.831 | 90.225 | 27.763 | 1.00 | 18.80 | 6 |
| 1394 | N | SER A 175 | 36.441 | 86.493 | 23.260 | 1.00 | 14.22 | 7 | 1436 | OD1 | ASP A 179 | 30.462 | 91.232 | 28.431 | 1.00 | 20.56 | 8 |
| 1395 | CA | SER A 175 | 37.710 | 87.093 | 23.770 | 1.00 | 16.89 | 6 | 1437 | OD2 | ASP A 179 | 30.213 | 89.893 | 26.753 | 1.00 | 13.51 | 8 |
| 1396 | C | SER A 175 | 37.712 | 87.131 | 25.231 | 1.00 | 18.02 | 6 | 1438 | N | ARG A 180 | 29.115 | 87.768 | 29.477 | 1.00 | 13.02 | 7 |
| 1397 | O | SER A 175 | 38.617 | 86.587 | 25.938 | 1.00 | 19.20 | 8 | 1439 | CA | ARG A 180 | 28.057 | 86.771 | 29.205 | 1.00 | 11.54 | 6 |
| 1398 | CB | SER A 175 | 37.868 | 88.470 | 23.138 | 1.00 | 17.86 | 6 | 1440 | C | ARG A 180 | 27.585 | 86.833 | 27.757 | 1.00 | 10.36 | 6 |
| 1399 | OG | SER A 175 | 39.049 | 89.044 | 23.724 | 1.00 | 24.28 | 8 | 1441 | O | ARG A 180 | 27.261 | 85.746 | 27.225 | 1.00 | 11.27 | 8 |
| 1400 | N | ASN A 176 | 36.650 | 87.662 | 25.854 | 1.00 | 14.39 | 7 | 1442 | CB | ARG A 180 | 26.893 | 87.051 | 30.172 | 1.00 | 13.31 | 6 |
| 1401 | CA | ASN A 176 | 36.515 | 87.678 | 27.336 | 1.00 | 13.41 | 6 | 1443 | CG | ARG A 180 | 27.286 | 86.796 | 31.654 | 1.00 | 12.49 | 6 |
| 1402 | C | ASN A 176 | 35.511 | 86.561 | 27.678 | 1.00 | 12.76 | 6 | 1444 | CD | ARG A 180 | 27.797 | 85.340 | 31.899 | 1.00 | 10.75 | 6 |
| 1403 | O | ASN A 176 | 34.286 | 86.760 | 27.482 | 1.00 | 13.43 | 8 | 1445 | NE | ARG A 180 | 26.694 | 84.389 | 31.571 | 1.00 | 11.38 | 7 |
| 1404 | CB | ASN A 176 | 35.898 | 89.032 | 27.724 | 1.00 | 15.61 | 6 | 1446 | CZ | ARG A 180 | 26.896 | 83.305 | 30.812 | 1.00 | 11.55 | 6 |
| 1405 | CG | ASN A 176 | 35.749 | 89.123 | 29.243 | 1.00 | 17.91 | 6 | 1447 | NH1 | ARG A 180 | 28.090 | 82.893 | 30.359 | 1.00 | 11.21 | 7 |
| 1406 | OD1 | ASN A 176 | 35.963 | 88.166 | 29.982 | 1.00 | 15.18 | 8 | 1448 | NH2 | ARG A 180 | 25.769 | 82.597 | 30.589 | 1.00 | 13.64 | 7 |
| 1407 | ND2 | ASN A 176 | 35.402 | 90.347 | 29.694 | 1.00 | 22.13 | 7 | 1449 | N | TYR A 181 | 27.508 | 87.990 | 27.113 | 1.00 | 10.51 | 7 |
| 1408 | N | TRP A 177 | 36.085 | 85.465 | 28.237 | 1.00 | 14.29 | 7 | 1450 | CA | TYR A 181 | 27.104 | 87.980 | 25.688 | 1.00 | 10.68 | 6 |
| 1409 | CA | TRP A 177 | 35.172 | 84.361 | 28.558 | 1.00 | 13.39 | 6 | 1451 | C | TYR A 181 | 28.195 | 87.277 | 24.870 | 1.00 | 11.14 | 6 |
| 1410 | O | TRP A 177 | 34.248 | 84.677 | 29.724 | 1.00 | 15.05 | 8 | 1452 | O | TYR A 181 | 27.826 | 86.403 | 24.044 | 1.00 | 10.66 | 8 |
| 1411 | C | TRP A 177 | 33.279 | 83.898 | 29.909 | 1.00 | 14.25 | 6 | 1453 | CB | TYR A 181 | 26.915 | 89.446 | 25.196 | 1.00 | 12.30 | 6 |
| 1412 | CB | TRP A 177 | 36.054 | 83.145 | 28.953 | 1.00 | 16.12 | 6 | 1454 | CG | TYR A 181 | 26.645 | 89.417 | 23.698 | 1.00 | 12.16 | 6 |
| 1413 | CG | TRP A 177 | 36.712 | 82.559 | 27.721 | 1.00 | 14.43 | 6 | 1455 | CD1 | TYR A 181 | 25.446 | 89.009 | 23.179 | 1.00 | 13.07 | 6 |
| 1414 | CD1 | TRP A 177 | 37.745 | 83.101 | 26.998 | 1.00 | 16.58 | 6 | 1456 | CD2 | TYR A 181 | 27.712 | 89.736 | 22.837 | 1.00 | 15.09 | 6 |
| 1415 | CD2 | TRP A 177 | 36.399 | 81.291 | 27.142 | 1.00 | 13.92 | 6 | 1457 | CE1 | TYR A 181 | 25.242 | 88.936 | 21.808 | 1.00 | 18.03 | 6 |
| 1416 | NE1 | TRP A 177 | 38.070 | 82.235 | 25.940 | 1.00 | 18.57 | 7 | 1458 | CE2 | TYR A 181 | 27.510 | 89.688 | 21.457 | 1.00 | 16.90 | 6 |
| 1417 | CE2 | TRP A 177 | 37.234 | 81.131 | 26.014 | 1.00 | 18.68 | 6 | 1459 | CZ | TYR A 181 | 26.275 | 89.265 | 20.988 | 1.00 | 19.76 | 6 |
| 1418 | CE3 | TRP A 177 | 35.437 | 80.298 | 27.392 | 1.00 | 17.34 | 6 | 1460 | OH | TYR A 181 | 26.097 | 89.156 | 19.614 | 1.00 | 17.30 | 8 |
| 1419 | CZ2 | TRP A 177 | 37.148 | 80.031 | 25.169 | 1.00 | 14.28 | 6 | 1461 | N | GLU A 182 | 29.473 | 87.528 | 25.083 | 1.00 | 13.50 | 7 |
| 1420 | CZ3 | TRP A 177 | 35.379 | 79.182 | 26.574 | 1.00 | 17.20 | 6 | 1462 | CA | GLU A 182 | 30.468 | 86.836 | 24.265 | 1.00 | 12.35 | 6 |
| 1421 | CH2 | TRP A 177 | 36.253 | 79.045 | 25.441 | 1.00 | 18.00 | 6 | 1463 | C | GLU A 182 | 30.442 | 85.311 | 24.504 | 1.00 | 10.45 | 6 |
| 1422 | N | ASP A 178 | 34.477 | 85.795 | 30.469 | 1.00 | 12.43 | 7 | 1464 | O | GLU A 182 | 30.482 | 84.533 | 23.582 | 1.00 | 11.45 | 8 |
| 1423 | CA | ASP A 178 | 33.507 | 86.126 | 31.517 | 1.00 | 11.08 | 6 | 1465 | CB | GLU A 182 | 31.939 | 87.266 | 24.571 | 1.00 | 10.48 | 6 |
| 1424 | C | ASP A 178 | 32.454 | 87.115 | 31.053 | 1.00 | 12.88 | 6 | 1466 | CG | GLU A 182 | 32.131 | 88.769 | 24.214 | 1.00 | 12.66 | 6 |
| 1425 | O | ASP A 178 | 31.586 | 87.420 | 31.881 | 1.00 | 15.73 | 8 | 1467 | CD | GLU A 182 | 33.640 | 89.046 | 24.246 | 1.00 | 19.30 | 6 |
| 1426 | CB | ASP A 178 | 34.243 | 86.717 | 32.739 | 1.00 | 17.78 | 6 | 1468 | OE1 | GLU A 182 | 34.487 | 88.229 | 23.958 | 1.00 | 15.48 | 8 |
| 1427 | CG | ASP A 178 | 35.201 | 85.739 | 33.362 | 1.00 | 24.33 | 6 | 1469 | OE2 | GLU A 182 | 34.009 | 90.199 | 24.690 | 1.00 | 30.95 | 8 |
| 1428 | OD1 | ASP A 178 | 34.916 | 84.535 | 33.440 | 1.00 | 18.07 | 8 | 1470 | N | ALA A 183 | 30.314 | 84.945 | 25.796 | 1.00 | 10.17 | 7 |
| 1429 | OD2 | ASP A 178 | 36.317 | 86.155 | 33.777 | 1.00 | 24.77 | 8 | 1471 | CA | ALA A 183 | 30.436 | 83.521 | 26.110 | 1.00 | 11.02 | 6 |
| 1430 | N | ASP A 179 | 32.527 | 87.608 | 29.810 | 1.00 | 11.79 | 7 | 1472 | C | ALA A 183 | 29.302 | 82.709 | 25.471 | 1.00 | 11.67 | 6 |
| 1431 | CA | ASP A 179 | 31.448 | 88.502 | 29.357 | 1.00 | 11.42 | 6 | 1473 | O | ALA A 183 | 29.555 | 81.542 | 25.197 | 1.00 | 10.91 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1474 | CB | ALA A 183 | 30.290 | 83.352 | 27.664 | 1.00 | 11.34 | 6 | 1516 | CA | PHE A 188 | 34.321 | 78.658 | 21.604 | 1.00 | 10.93 | 6 |
| 1475 | N | GLN A 184 | 28.196 | 83.381 | 25.172 | 1.00 | 10.70 | 7 | 1517 | C | PHE A 188 | 35.600 | 78.457 | 20.806 | 1.00 | 13.95 | 6 |
| 1476 | CA | GLN A 184 | 27.046 | 82.624 | 24.601 | 1.00 | 8.62 | 6 | 1518 | O | PHE A 188 | 35.534 | 78.128 | 19.632 | 1.00 | 13.55 | 8 |
| 1477 | C | GLN A 184 | 26.939 | 82.844 | 23.102 | 1.00 | 10.69 | 6 | 1519 | CB | PHE A 188 | 33.682 | 77.259 | 21.822 | 1.00 | 11.05 | 6 |
| 1478 | O | GLN A 184 | 26.509 | 81.913 | 22.388 | 1.00 | 10.72 | 8 | 1520 | CG | PHE A 188 | 34.177 | 76.552 | 23.071 | 1.00 | 11.08 | 6 |
| 1479 | CB | GLN A 184 | 25.772 | 83.078 | 25.330 | 1.00 | 12.35 | 6 | 1521 | CD1 | PHE A 188 | 35.431 | 75.953 | 23.060 | 1.00 | 14.39 | 6 |
| 1480 | CG | GLN A 184 | 25.730 | 82.584 | 26.785 | 1.00 | 9.80 | 6 | 1522 | CD2 | PHE A 188 | 33.364 | 76.492 | 24.194 | 1.00 | 14.52 | 6 |
| 1481 | CD | GLN A 184 | 24.603 | 83.315 | 27.538 | 1.00 | 12.56 | 6 | 1523 | CE1 | PHE A 188 | 35.865 | 75.309 | 24.204 | 1.00 | 15.63 | 6 |
| 1482 | OE1 | GLN A 184 | 24.739 | 84.527 | 27.890 | 1.00 | 15.21 | 8 | 1524 | CE2 | PHE A 188 | 33.821 | 75.818 | 25.327 | 1.00 | 14.28 | 6 |
| 1483 | NE2 | GLN A 184 | 23.536 | 82.580 | 27.775 | 1.00 | 8.78 | 7 | 1525 | CZ | PHE A 188 | 35.081 | 75.233 | 25.350 | 1.00 | 12.75 | 6 |
| 1484 | N | TRP A 185 | 27.186 | 84.018 | 22.585 | 1.00 | 11.90 | 7 | 1526 | N | THR A 189 | 36.737 | 78.710 | 21.504 | 1.00 | 11.89 | 7 |
| 1485 | CA | TRP A 185 | 26.968 | 84.285 | 21.148 | 1.00 | 9.74 | 6 | 1527 | CA | THR A 189 | 38.000 | 78.578 | 20.769 | 1.00 | 11.77 | 6 |
| 1486 | C | TRP A 185 | 28.252 | 84.298 | 20.318 | 1.00 | 10.30 | 6 | 1528 | C | THR A 189 | 38.851 | 77.524 | 21.457 | 1.00 | 13.65 | 6 |
| 1487 | O | TRP A 185 | 28.093 | 84.277 | 19.065 | 1.00 | 11.67 | 8 | 1529 | O | THR A 189 | 38.630 | 77.149 | 22.589 | 1.00 | 14.67 | 8 |
| 1488 | CB | TRP A 185 | 26.201 | 85.647 | 20.965 | 1.00 | 12.61 | 6 | 1530 | CB | THR A 189 | 38.826 | 79.904 | 20.788 | 1.00 | 12.56 | 6 |
| 1489 | CG | TRP A 185 | 24.696 | 85.390 | 21.039 | 1.00 | 10.95 | 6 | 1531 | OG1 | THR A 189 | 39.066 | 80.215 | 22.180 | 1.00 | 15.52 | 8 |
| 1490 | CD1 | TRP A 185 | 23.863 | 85.166 | 19.989 | 1.00 | 12.59 | 6 | 1532 | CG2 | THR A 189 | 38.012 | 81.045 | 20.136 | 1.00 | 13.79 | 6 |
| 1491 | CD2 | TRP A 185 | 23.898 | 85.345 | 22.226 | 1.00 | 12.07 | 6 | 1533 | N | ASP A 190 | 39.773 | 76.961 | 20.639 | 1.00 | 11.10 | 7 |
| 1492 | NE1 | TRP A 185 | 22.561 | 84.887 | 20.428 | 1.00 | 14.15 | 7 | 1534 | CA | ASP A 190 | 40.736 | 75.985 | 21.186 | 1.00 | 11.48 | 6 |
| 1493 | CE2 | TRP A 185 | 22.600 | 85.003 | 21.805 | 1.00 | 13.63 | 6 | 1535 | C | ASP A 190 | 42.109 | 76.575 | 20.929 | 1.00 | 11.63 | 6 |
| 1494 | CE3 | TRP A 185 | 24.154 | 85.530 | 23.587 | 1.00 | 13.34 | 6 | 1536 | O | ASP A 190 | 42.403 | 77.103 | 19.861 | 1.00 | 13.03 | 8 |
| 1495 | CZ2 | TRP A 185 | 21.534 | 84.846 | 22.703 | 1.00 | 14.01 | 6 | 1537 | CB | ASP A 190 | 40.530 | 74.703 | 20.365 | 1.00 | 11.07 | 6 |
| 1496 | CE2 | TRP A 185 | 23.093 | 85.361 | 24.494 | 1.00 | 14.75 | 6 | 1538 | CB | ASP A 190 | 41.445 | 73.591 | 20.781 | 1.00 | 12.55 | 6 |
| 1497 | CH2 | TRP A 185 | 21.812 | 85.004 | 24.035 | 1.00 | 13.91 | 6 | 1539 | OD1 | ASP A 190 | 42.691 | 73.716 | 20.943 | 1.00 | 14.12 | 8 |
| 1498 | N | LYS A 186 | 29.413 | 84.254 | 20.924 | 1.00 | 11.31 | 7 | 1540 | OD2 | ASP A 190 | 40.937 | 72.422 | 20.956 | 1.00 | 14.32 | 8 |
| 1499 | CA | LYS A 186 | 30.655 | 84.170 | 20.127 | 1.00 | 12.29 | 6 | 1541 | N | PRO A 191 | 43.013 | 76.539 | 21.885 | 1.00 | 12.39 | 7 |
| 1500 | C | LYS A 186 | 31.228 | 82.764 | 20.238 | 1.00 | 14.72 | 6 | 1542 | CA | PRO A 191 | 44.344 | 77.094 | 21.756 | 1.00 | 16.15 | 6 |
| 1501 | O | LYS A 186 | 30.718 | 81.896 | 20.981 | 1.00 | 12.47 | 8 | 1543 | C | PRO A 191 | 45.205 | 76.488 | 20.648 | 1.00 | 17.03 | 6 |
| 1502 | CB | LYS A 186 | 31.682 | 85.224 | 20.582 | 1.00 | 11.09 | 6 | 1544 | O | PRO A 191 | 46.194 | 77.139 | 20.258 | 1.00 | 17.33 | 8 |
| 1503 | CG | LYS A 186 | 31.145 | 86.646 | 20.243 | 1.00 | 14.74 | 6 | 1545 | CB | PRO A 191 | 45.077 | 76.806 | 23.067 | 1.00 | 15.82 | 6 |
| 1504 | CD | LYS A 186 | 32.295 | 87.655 | 20.601 | 1.00 | 14.53 | 6 | 1546 | CG | PRO A 191 | 43.951 | 76.489 | 24.024 | 1.00 | 19.99 | 6 |
| 1505 | CE | LYS A 186 | 31.688 | 89.051 | 20.286 | 1.00 | 20.29 | 6 | 1547 | CD | PRO A 191 | 42.769 | 75.960 | 23.220 | 1.00 | 15.14 | 6 |
| 1506 | NZ | LYS A 186 | 32.744 | 89.943 | 19.726 | 1.00 | 28.67 | 7 | 1548 | N | ALA A 192 | 44.778 | 75.374 | 20.102 | 1.00 | 12.41 | 7 |
| 1507 | N | ASN A 187 | 32.217 | 82.446 | 19.379 | 1.00 | 13.16 | 7 | 1549 | CA | ALA A 192 | 45.446 | 74.851 | 18.871 | 1.00 | 16.29 | 6 |
| 1508 | CA | ASN A 187 | 32.653 | 81.074 | 19.195 | 1.00 | 13.22 | 6 | 1550 | C | ALA A 192 | 45.279 | 75.807 | 17.697 | 1.00 | 21.11 | 6 |
| 1509 | C | ASN A 187 | 33.587 | 80.604 | 20.314 | 1.00 | 15.43 | 6 | 1551 | O | ALA A 192 | 46.014 | 75.779 | 16.675 | 1.00 | 19.85 | 8 |
| 1510 | O | ASN A 187 | 34.587 | 81.250 | 20.646 | 1.00 | 12.76 | 8 | 1552 | CB | ALA A 192 | 44.978 | 73.466 | 18.579 | 1.00 | 20.48 | 6 |
| 1511 | CB | ASN A 187 | 33.386 | 80.850 | 17.862 | 1.00 | 12.72 | 6 | 1553 | N | GLY A 193 | 44.317 | 76.695 | 17.671 | 1.00 | 16.93 | 7 |
| 1512 | CG | ASN A 187 | 32.673 | 81.537 | 16.697 | 1.00 | 18.84 | 6 | 1554 | CA | GLY A 193 | 44.199 | 77.733 | 16.641 | 1.00 | 17.03 | 6 |
| 1513 | OD1 | ASN A 187 | 31.447 | 81.456 | 16.631 | 1.00 | 15.46 | 8 | 1555 | C | GLY A 193 | 42.919 | 77.582 | 15.819 | 1.00 | 17.85 | 6 |
| 1514 | ND2 | ASN A 187 | 33.426 | 82.219 | 15.839 | 1.00 | 16.94 | 7 | 1556 | O | GLY A 193 | 42.991 | 77.960 | 14.651 | 1.00 | 17.03 | 8 |
| 1515 | N | PHE A 188 | 33.369 | 79.356 | 20.719 | 1.00 | 11.91 | 7 | 1557 | N | PHE A 194 | 41.888 | 76.955 | 16.373 | 1.00 | 13.47 | 7 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1558 | CA | PHE A 194 | 40.612 | 76.976 | 15.567 | 1.00 | 11.84 | 6 | 1600 | CG | LEU A 199 | 25.178 | 74.135 | 16.526 | 1.00 | 10.88 | 6 |
| 1559 | C | PHE A 194 | 39.441 | 77.265 | 16.536 | 1.00 | 11.03 | 6 | 1601 | CD1 | LEU A 199 | 24.799 | 72.879 | 17.321 | 1.00 | 12.59 | 6 |
| 1560 | O | PHE A 194 | 39.621 | 77.423 | 17.750 | 1.00 | 11.69 | 8 | 1602 | CD2 | LEU A 199 | 24.658 | 74.045 | 15.071 | 1.00 | 14.19 | 6 |
| 1561 | CB | PHE A 194 | 40.411 | 75.629 | 14.855 | 1.00 | 10.98 | 6 | 1603 | N | SER A 200 | 23.024 | 78.144 | 16.505 | 1.00 | 11.57 | 7 |
| 1562 | CG | PHE A 194 | 40.568 | 74.412 | 15.767 | 1.00 | 11.46 | 6 | 1604 | CA | SER A 200 | 22.055 | 79.160 | 16.950 | 1.00 | 10.26 | 6 |
| 1563 | CD1 | PHE A 194 | 39.545 | 74.063 | 16.649 | 1.00 | 11.56 | 6 | 1605 | C | SER A 200 | 20.810 | 78.424 | 17.499 | 1.00 | 11.50 | 6 |
| 1564 | CD2 | PHE A 194 | 41.707 | 73.656 | 15.747 | 1.00 | 15.24 | 6 | 1606 | O | SER A 200 | 19.994 | 77.917 | 16.741 | 1.00 | 11.79 | 8 |
| 1565 | CE1 | PHE A 194 | 39.688 | 72.942 | 17.460 | 1.00 | 11.26 | 6 | 1607 | CB | SER A 200 | 21.636 | 80.012 | 15.731 | 1.00 | 14.77 | 6 |
| 1566 | CE2 | PHE A 194 | 41.871 | 72.533 | 16.574 | 1.00 | 12.49 | 6 | 1608 | OG | SER A 200 | 20.723 | 81.011 | 16.249 | 1.00 | 13.69 | 8 |
| 1567 | CZ | PHE A 194 | 40.860 | 72.181 | 17.450 | 1.00 | 12.03 | 6 | 1609 | N | GLN A 201 | 20.786 | 78.294 | 18.837 | 1.00 | 10.61 | 7 |
| 1568 | N | SER A 195 | 38.283 | 77.497 | 15.895 | 1.00 | 10.73 | 7 | 1610 | CA | GLN A 201 | 19.599 | 77.668 | 19.473 | 1.00 | 11.55 | 6 |
| 1569 | CA | SER A 195 | 37.097 | 77.782 | 16.704 | 1.00 | 11.52 | 6 | 1611 | C | GLN A 201 | 18.421 | 78.648 | 19.371 | 1.00 | 11.79 | 6 |
| 1570 | C | SER A 195 | 36.081 | 76.649 | 16.423 | 1.00 | 11.92 | 6 | 1612 | O | GLN A 201 | 17.305 | 78.161 | 19.700 | 1.00 | 12.43 | 8 |
| 1571 | O | SER A 195 | 36.284 | 75.902 | 15.519 | 1.00 | 10.36 | 8 | 1613 | CB | GLN A 201 | 19.852 | 77.359 | 20.969 | 1.00 | 11.94 | 6 |
| 1572 | CB | SER A 195 | 36.416 | 79.059 | 16.186 | 1.00 | 16.30 | 6 | 1614 | CG | GLN A 201 | 21.042 | 76.370 | 21.151 | 1.00 | 10.05 | 6 |
| 1573 | OG | SER A 195 | 37.442 | 80.119 | 16.216 | 1.00 | 22.79 | 8 | 1615 | CD | GLN A 201 | 22.393 | 77.086 | 21.126 | 1.00 | 10.84 | 6 |
| 1574 | N | LEU A 196 | 35.060 | 76.594 | 17.262 | 1.00 | 12.22 | 7 | 1616 | OE1 | GLN A 201 | 22.499 | 78.298 | 21.208 | 1.00 | 11.60 | 8 |
| 1575 | CA | LEU A 196 | 34.007 | 75.622 | 17.060 | 1.00 | 12.16 | 6 | 1617 | NE2 | GLN A 201 | 23.465 | 76.231 | 21.079 | 1.00 | 9.83 | 7 |
| 1576 | C | LEU A 196 | 32.756 | 76.384 | 16.584 | 1.00 | 7.60 | 6 | 1618 | N | GLU A 202 | 18.590 | 79.860 | 18.862 | 1.00 | 10.41 | 7 |
| 1577 | O | LEU A 196 | 32.384 | 77.416 | 17.112 | 1.00 | 13.16 | 8 | 1619 | CA | GLU A 202 | 17.434 | 80.763 | 18.667 | 1.00 | 11.55 | 6 |
| 1578 | CB | LEU A 196 | 33.660 | 74.883 | 18.410 | 1.00 | 10.95 | 6 | 1620 | C | GLU A 202 | 16.849 | 80.531 | 17.277 | 1.00 | 14.51 | 6 |
| 1579 | CG | LEU A 196 | 34.880 | 74.298 | 19.107 | 1.00 | 10.75 | 6 | 1621 | O | GLU A 202 | 15.856 | 81.166 | 16.903 | 1.00 | 16.57 | 8 |
| 1580 | CD1 | LEU A 196 | 34.439 | 73.454 | 20.334 | 1.00 | 11.59 | 6 | 1622 | CB | GLU A 202 | 17.877 | 82.226 | 18.875 | 1.00 | 10.69 | 6 |
| 1581 | CD2 | LEU A 196 | 35.719 | 73.384 | 18.134 | 1.00 | 12.48 | 6 | 1623 | CG | GLU A 202 | 18.522 | 82.442 | 20.252 | 1.00 | 9.01 | 6 |
| 1582 | N | ALA A 197 | 32.139 | 75.877 | 15.481 | 1.00 | 9.97 | 7 | 1624 | CD | GLU A 202 | 20.002 | 82.069 | 20.330 | 1.00 | 12.78 | 6 |
| 1583 | CA | ALA A 197 | 30.995 | 76.637 | 14.905 | 1.00 | 10.64 | 6 | 1625 | OE1 | GLU A 202 | 20.680 | 82.031 | 19.299 | 1.00 | 16.62 | 8 |
| 1584 | C | ALA A 197 | 29.788 | 76.658 | 15.830 | 1.00 | 14.16 | 6 | 1626 | OE2 | GLU A 202 | 20.457 | 81.782 | 21.434 | 1.00 | 12.31 | 8 |
| 1585 | O | ALA A 197 | 29.362 | 75.622 | 16.314 | 1.00 | 11.22 | 8 | 1627 | N | ASN A 203 | 17.507 | 79.704 | 16.435 | 1.00 | 11.04 | 7 |
| 1586 | CB | ALA A 197 | 30.629 | 75.928 | 13.565 | 1.00 | 10.95 | 6 | 1628 | CA | ASN A 203 | 16.939 | 79.318 | 15.142 | 1.00 | 10.64 | 6 |
| 1587 | N | ASP A 198 | 29.429 | 77.869 | 16.236 | 1.00 | 10.28 | 7 | 1629 | C | ASN A 203 | 16.020 | 78.098 | 15.372 | 1.00 | 13.48 | 6 |
| 1588 | CA | ASP A 198 | 28.459 | 78.009 | 17.350 | 1.00 | 10.50 | 6 | 1630 | O | ASN A 203 | 16.441 | 77.148 | 16.008 | 1.00 | 12.81 | 8 |
| 1589 | C | ASP A 198 | 27.030 | 77.880 | 16.795 | 1.00 | 11.99 | 6 | 1631 | CB | ASN A 203 | 18.105 | 78.892 | 14.217 | 1.00 | 11.71 | 6 |
| 1590 | O | ASP A 198 | 26.607 | 78.731 | 15.993 | 1.00 | 13.33 | 8 | 1632 | CG | ASN A 203 | 17.604 | 78.307 | 12.930 | 1.00 | 15.36 | 6 |
| 1591 | CB | ASP A 198 | 28.744 | 79.433 | 17.900 | 1.00 | 12.29 | 6 | 1633 | OD1 | ASN A 203 | 17.271 | 77.124 | 12.838 | 1.00 | 15.37 | 8 |
| 1592 | CG | ASP A 198 | 28.236 | 79.529 | 19.353 | 1.00 | 10.72 | 6 | 1634 | ND2 | ASN A 203 | 17.611 | 79.108 | 11.829 | 1.00 | 15.33 | 7 |
| 1593 | OD1 | ASP A 198 | 28.683 | 78.683 | 20.172 | 1.00 | 11.33 | 8 | 1635 | N | GLY A 204 | 14.797 | 78.219 | 14.831 | 1.00 | 13.94 | 7 |
| 1594 | OD2 | ASP A 198 | 27.401 | 80.452 | 19.671 | 1.00 | 10.45 | 8 | 1636 | CA | GLY A 204 | 13.813 | 77.115 | 15.175 | 1.00 | 14.96 | 6 |
| 1595 | N | LEU A 199 | 26.310 | 76.847 | 17.247 | 1.00 | 10.29 | 7 | 1637 | C | GLY A 204 | 14.202 | 75.766 | 14.593 | 1.00 | 12.98 | 6 |
| 1596 | CA | LEU A 199 | 24.927 | 76.690 | 16.763 | 1.00 | 8.80 | 6 | 1638 | O | GLY A 204 | 13.891 | 74.775 | 15.243 | 1.00 | 14.33 | 8 |
| 1597 | C | LEU A 199 | 24.086 | 77.821 | 17.321 | 1.00 | 9.88 | 6 | 1639 | N | THR A 205 | 14.802 | 75.705 | 13.401 | 1.00 | 11.88 | 7 |
| 1598 | O | LEU A 199 | 24.246 | 78.320 | 18.449 | 1.00 | 11.27 | 8 | 1640 | CA | THR A 205 | 15.279 | 74.405 | 12.894 | 1.00 | 12.45 | 6 |
| 1599 | CB | LEU A 199 | 24.452 | 75.296 | 17.279 | 1.00 | 9.52 | 6 | 1641 | C | THR A 205 | 16.275 | 73.780 | 13.856 | 1.00 | 11.35 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1642 | O | THR A 205 | 16.161 | 72.621 | 14.172 | 1.00 | 11.84 | 8 | 1684 | CB | LEU A 210 | 19.388 | 70.688 | 19.713 | 1.00 | 10.40 | 6 |
| 1643 | CB | THR A 205 | 15.865 | 74.603 | 11.497 | 1.00 | 14.40 | 6 | 1685 | CG | LEU A 210 | 20.603 | 71.237 | 18.893 | 1.00 | 10.20 | 6 |
| 1644 | OG1 | THR A 205 | 14.760 | 75.060 | 10.662 | 1.00 | 18.35 | 8 | 1686 | CD1 | LEU A 210 | 20.918 | 72.628 | 19.480 | 1.00 | 12.47 | 6 |
| 1645 | CG2 | THR A 205 | 16.344 | 73.256 | 10.930 | 1.00 | 16.31 | 6 | 1687 | CD2 | LEU A 210 | 21.766 | 70.260 | 18.920 | 1.00 | 13.21 | 6 |
| 1646 | N | ILE A 206 | 17.295 | 74.586 | 14.188 | 1.00 | 10.89 | 7 | 1688 | N | THR A 211 | 16.539 | 69.327 | 20.069 | 1.00 | 9.66 | 7 |
| 1647 | CA | ILE A 206 | 18.330 | 73.996 | 15.081 | 1.00 | 10.54 | 6 | 1689 | CA | THR A 211 | 15.520 | 68.689 | 20.933 | 1.00 | 11.98 | 6 |
| 1648 | C | ILE A 206 | 17.736 | 73.689 | 16.457 | 1.00 | 9.48 | 6 | 1690 | C | THR A 211 | 15.294 | 67.272 | 20.496 | 1.00 | 11.93 | 6 |
| 1649 | O | ILE A 206 | 18.081 | 72.638 | 17.051 | 1.00 | 10.61 | 8 | 1691 | O | THR A 211 | 15.311 | 66.354 | 21.335 | 1.00 | 11.42 | 8 |
| 1650 | CB | ILE A 206 | 19.481 | 75.017 | 15.212 | 1.00 | 9.16 | 6 | 1692 | CB | THR A 211 | 14.193 | 69.502 | 20.889 | 1.00 | 12.29 | 6 |
| 1651 | CG1 | ILE A 206 | 20.193 | 75.155 | 13.844 | 1.00 | 12.29 | 6 | 1693 | OG1 | THR A 211 | 14.488 | 70.842 | 21.373 | 1.00 | 11.73 | 8 |
| 1652 | CG2 | ILE A 206 | 20.550 | 74.624 | 16.273 | 1.00 | 11.91 | 6 | 1694 | CG2 | THR A 211 | 13.137 | 68.832 | 21.808 | 1.00 | 10.37 | 6 |
| 1653 | CD1 | ILE A 206 | 20.691 | 73.847 | 13.218 | 1.00 | 12.69 | 6 | 1695 | N | ASP A 212 | 15.071 | 67.084 | 19.170 | 1.00 | 12.47 | 7 |
| 1654 | N | ALA A 207 | 16.912 | 74.562 | 17.021 | 1.00 | 10.30 | 7 | 1696 | CA | ASP A 212 | 14.813 | 65.738 | 18.671 | 1.00 | 10.73 | 6 |
| 1655 | CA | ALA A 207 | 16.350 | 74.185 | 18.339 | 1.00 | 12.45 | 6 | 1697 | C | ASP A 212 | 15.998 | 64.812 | 18.997 | 1.00 | 12.42 | 6 |
| 1656 | C | ALA A 207 | 15.583 | 72.871 | 18.311 | 1.00 | 12.45 | 6 | 1698 | O | ASP A 212 | 15.748 | 63.598 | 19.194 | 1.00 | 12.22 | 8 |
| 1657 | O | ALA A 207 | 15.714 | 72.053 | 19.217 | 1.00 | 13.37 | 8 | 1699 | CB | ASP A 212 | 14.605 | 65.829 | 17.159 | 1.00 | 12.33 | 6 |
| 1658 | CB | ALA A 207 | 15.511 | 75.359 | 18.883 | 1.00 | 13.30 | 6 | 1700 | CG | ASP A 212 | 13.253 | 66.477 | 16.797 | 1.00 | 15.18 | 6 |
| 1659 | N | GLN A 208 | 14.749 | 72.676 | 17.282 | 1.00 | 10.55 | 7 | 1701 | OD1 | ASP A 212 | 12.379 | 66.643 | 17.667 | 1.00 | 13.61 | 8 |
| 1660 | CA | GLN A 208 | 13.968 | 71.431 | 17.236 | 1.00 | 11.60 | 6 | 1702 | OD2 | ASP A 212 | 13.100 | 66.828 | 15.585 | 1.00 | 14.64 | 8 |
| 1661 | C | GLN A 208 | 14.842 | 70.256 | 16.877 | 1.00 | 14.22 | 6 | 1703 | N | ALA A 213 | 17.230 | 65.326 | 18.830 | 1.00 | 10.02 | 7 |
| 1662 | O | GLN A 208 | 14.627 | 69.200 | 17.426 | 1.00 | 11.79 | 8 | 1704 | CA | ALA A 213 | 18.376 | 64.422 | 19.084 | 1.00 | 10.72 | 6 |
| 1663 | CB | GLN A 208 | 12.869 | 71.573 | 16.136 | 1.00 | 13.62 | 6 | 1705 | C | ALA A 213 | 18.422 | 64.023 | 20.552 | 1.00 | 10.18 | 6 |
| 1664 | CG | GLN A 208 | 11.847 | 70.429 | 16.197 | 1.00 | 14.37 | 6 | 1706 | O | ALA A 213 | 18.819 | 62.882 | 20.861 | 1.00 | 11.96 | 8 |
| 1665 | CD | GLN A 208 | 11.089 | 70.392 | 17.513 | 1.00 | 15.09 | 6 | 1707 | CB | ALA A 213 | 19.679 | 65.163 | 18.735 | 1.00 | 10.83 | 6 |
| 1666 | OE1 | GLN A 208 | 10.565 | 71.371 | 17.957 | 1.00 | 14.67 | 8 | 1708 | N | ALA A 214 | 18.155 | 64.970 | 21.448 | 1.00 | 12.55 | 7 |
| 1667 | NE2 | GLN A 208 | 11.168 | 69.230 | 18.180 | 1.00 | 14.23 | 7 | 1709 | CA | ALA A 214 | 18.185 | 64.599 | 22.892 | 1.00 | 10.81 | 6 |
| 1668 | N | TYR A 209 | 15.876 | 70.454 | 16.062 | 1.00 | 11.41 | 7 | 1710 | C | ALA A 214 | 17.073 | 63.631 | 23.235 | 1.00 | 11.35 | 6 |
| 1669 | CA | TYR A 209 | 16.807 | 69.372 | 15.724 | 1.00 | 10.71 | 6 | 1711 | O | ALA A 214 | 17.246 | 62.667 | 23.953 | 1.00 | 12.75 | 8 |
| 1670 | C | TYR A 209 | 17.570 | 68.930 | 16.979 | 1.00 | 10.31 | 6 | 1712 | CB | ALA A 214 | 18.038 | 65.876 | 23.757 | 1.00 | 10.21 | 6 |
| 1671 | O | TYR A 209 | 17.634 | 67.727 | 17.231 | 1.00 | 11.12 | 8 | 1713 | N | VAL A 215 | 15.885 | 63.854 | 22.677 | 1.00 | 10.82 | 7 |
| 1672 | CB | TYR A 209 | 17.840 | 69.989 | 14.743 | 1.00 | 11.54 | 6 | 1714 | CA | VAL A 215 | 14.724 | 62.923 | 22.875 | 1.00 | 11.60 | 6 |
| 1673 | CG | TYR A 209 | 19.072 | 69.148 | 14.457 | 1.00 | 12.56 | 6 | 1715 | C | VAL A 215 | 15.035 | 61.577 | 22.302 | 1.00 | 13.68 | 6 |
| 1674 | CD1 | TYR A 209 | 19.031 | 68.083 | 13.584 | 1.00 | 11.38 | 6 | 1716 | O | VAL A 215 | 14.673 | 60.552 | 22.903 | 1.00 | 15.03 | 8 |
| 1675 | CD2 | TYR A 209 | 20.269 | 69.485 | 15.060 | 1.00 | 12.87 | 6 | 1717 | CB | VAL A 215 | 13.462 | 63.523 | 22.283 | 1.00 | 14.89 | 6 |
| 1676 | CE1 | TYR A 209 | 20.184 | 67.341 | 13.286 | 1.00 | 16.27 | 6 | 1718 | CG1 | VAL A 215 | 12.285 | 62.514 | 22.234 | 1.00 | 16.68 | 6 |
| 1677 | CE2 | TYR A 209 | 21.432 | 68.739 | 14.794 | 1.00 | 13.55 | 6 | 1719 | CG2 | VAL A 215 | 12.982 | 64.740 | 23.099 | 1.00 | 15.78 | 6 |
| 1678 | CZ | TYR A 209 | 21.368 | 67.676 | 13.915 | 1.00 | 13.50 | 6 | 1720 | N | GLN A 216 | 15.759 | 61.496 | 21.193 | 1.00 | 12.25 | 7 |
| 1679 | OH | TYR A 209 | 22.527 | 66.968 | 13.654 | 1.00 | 14.21 | 8 | 1721 | CA | GLN A 216 | 16.153 | 60.192 | 20.632 | 1.00 | 13.52 | 6 |
| 1680 | N | LEU A 210 | 17.985 | 69.883 | 17.821 | 1.00 | 10.88 | 7 | 1722 | C | GLN A 216 | 17.023 | 59.404 | 21.577 | 1.00 | 13.62 | 6 |
| 1681 | CA | LEU A 210 | 18.731 | 69.461 | 19.027 | 1.00 | 10.76 | 6 | 1723 | O | GLN A 216 | 16.864 | 58.192 | 21.706 | 1.00 | 12.75 | 8 |
| 1682 | C | LEU A 210 | 17.776 | 68.829 | 20.049 | 1.00 | 11.52 | 6 | 1724 | CB | GLN A 216 | 16.814 | 60.382 | 19.232 | 1.00 | 12.82 | 6 |
| 1683 | O | LEU A 210 | 18.178 | 67.863 | 20.687 | 1.00 | 11.55 | 8 | 1725 | CG | GLN A 216 | 17.225 | 59.032 | 18.639 | 1.00 | 14.36 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 1726 | CD | GLN A 216 | 17.856 | 59.162 | 17.261 | 1.00 | 18.32 | 6 | 1768 | N | ASP A 223 | 19.009 | 57.376 | 30.709 | 1.00 | 11.67 | 7 |
| 1727 | OE1 | GLN A 216 | 18.762 | 59.976 | 16.980 | 1.00 | 21.98 | 8 | 1769 | CA | ASP A 223 | 18.391 | 57.768 | 31.951 | 1.00 | 10.83 | 6 |
| 1728 | NE2 | GLN A 216 | 17.392 | 58.348 | 16.335 | 1.00 | 19.07 | 7 | 1770 | C | ASP A 223 | 18.621 | 59.249 | 32.306 | 1.00 | 12.58 | 6 |
| 1729 | N | LEU A 217 | 17.996 | 60.043 | 22.269 | 1.00 | 11.16 | 7 | 1771 | O | ASP A 223 | 18.116 | 59.667 | 33.356 | 1.00 | 11.47 | 8 |
| 1730 | CA | LEU A 217 | 18.781 | 59.317 | 23.261 | 1.00 | 11.02 | 6 | 1772 | CB | ASP A 223 | 18.997 | 56.964 | 33.123 | 1.00 | 9.67 | 6 |
| 1731 | C | LEU A 217 | 17.885 | 58.756 | 24.396 | 1.00 | 10.47 | 6 | 1773 | CG | ASP A 223 | 18.744 | 55.469 | 32.925 | 1.00 | 12.72 | 6 |
| 1732 | O | LEU A 217 | 18.106 | 57.631 | 24.754 | 1.00 | 13.19 | 8 | 1774 | OD1 | ASP A 223 | 17.554 | 55.095 | 33.224 | 1.00 | 15.35 | 8 |
| 1733 | CB | LEU A 217 | 19.847 | 60.252 | 23.876 | 1.00 | 12.00 | 6 | 1775 | OD2 | ASP A 223 | 19.610 | 54.686 | 32.482 | 1.00 | 10.77 | 8 |
| 1734 | CG | LEU A 217 | 20.974 | 60.577 | 22.859 | 1.00 | 10.07 | 6 | 1776 | N | GLY A 224 | 19.186 | 59.972 | 31.348 | 1.00 | 11.00 | 7 |
| 1735 | CD1 | LEU A 217 | 21.770 | 61.789 | 23.418 | 1.00 | 10.56 | 6 | 1777 | CA | GLY A 224 | 19.393 | 61.413 | 31.651 | 1.00 | 11.62 | 6 |
| 1736 | CD2 | LEU A 217 | 21.953 | 59.383 | 22.787 | 1.00 | 12.18 | 6 | 1778 | C | GLY A 224 | 20.641 | 61.861 | 30.809 | 1.00 | 9.62 | 6 |
| 1737 | N | VAL A 218 | 16.940 | 59.584 | 24.844 | 1.00 | 10.50 | 7 | 1779 | O | GLY A 224 | 21.069 | 61.107 | 29.928 | 1.00 | 9.69 | 8 |
| 1738 | CA | VAL A 218 | 16.027 | 59.030 | 25.884 | 1.00 | 14.12 | 6 | 1780 | N | LEU A 225 | 20.869 | 63.123 | 30.983 | 1.00 | 10.32 | 7 |
| 1739 | C | VAL A 218 | 15.114 | 57.918 | 25.304 | 1.00 | 12.90 | 6 | 1781 | CA | LEU A 225 | 21.962 | 63.749 | 30.177 | 1.00 | 9.63 | 6 |
| 1740 | O | VAL A 218 | 14.914 | 56.898 | 25.978 | 1.00 | 14.29 | 8 | 1782 | C | LEU A 225 | 22.828 | 64.566 | 31.128 | 1.00 | 10.99 | 6 |
| 1741 | CB | VAL A 218 | 15.121 | 60.168 | 26.376 | 1.00 | 11.91 | 6 | 1783 | O | LEU A 225 | 22.356 | 65.110 | 32.097 | 1.00 | 10.86 | 8 |
| 1742 | CG1 | VAL A 218 | 14.131 | 59.671 | 27.428 | 1.00 | 14.89 | 6 | 1784 | CB | LEU A 225 | 21.389 | 64.780 | 29.172 | 1.00 | 9.89 | 6 |
| 1743 | CG2 | VAL A 218 | 16.045 | 61.169 | 27.107 | 1.00 | 14.59 | 6 | 1785 | CG | LEU A 225 | 20.424 | 64.212 | 28.122 | 1.00 | 10.00 | 6 |
| 1744 | N | ALA A 219 | 14.717 | 57.992 | 24.051 | 1.00 | 14.93 | 7 | 1786 | CD1 | LEU A 225 | 19.806 | 65.361 | 27.279 | 1.00 | 12.69 | 6 |
| 1745 | CA | ALA A 219 | 13.868 | 56.915 | 23.478 | 1.00 | 14.21 | 6 | 1787 | CD2 | LEU A 225 | 21.003 | 63.092 | 27.243 | 1.00 | 13.97 | 6 |
| 1746 | C | ALA A 219 | 14.647 | 55.619 | 23.377 | 1.00 | 16.64 | 6 | 1788 | N | ARG A 226 | 24.135 | 64.671 | 30.790 | 1.00 | 10.52 | 7 |
| 1747 | O | ALA A 219 | 14.072 | 54.517 | 23.401 | 1.00 | 14.94 | 8 | 1789 | CA | ARG A 226 | 24.993 | 65.777 | 31.295 | 1.00 | 9.01 | 6 |
| 1748 | CB | ALA A 219 | 13.379 | 57.270 | 22.059 | 1.00 | 15.54 | 6 | 1790 | C | ARG A 226 | 25.093 | 66.744 | 30.110 | 1.00 | 10.97 | 6 |
| 1749 | N | HIS A 220 | 15.959 | 55.702 | 23.258 | 1.00 | 12.54 | 7 | 1791 | O | ARG A 226 | 25.628 | 66.348 | 29.083 | 1.00 | 10.94 | 8 |
| 1750 | CA | HIS A 220 | 16.853 | 54.570 | 23.215 | 1.00 | 14.41 | 6 | 1792 | CB | ARG A 226 | 26.337 | 65.159 | 31.691 | 1.00 | 9.10 | 6 |
| 1751 | C | HIS A 220 | 17.305 | 54.124 | 24.611 | 1.00 | 12.25 | 6 | 1793 | CG | ARG A 226 | 27.381 | 66.213 | 32.158 | 1.00 | 8.52 | 6 |
| 1752 | O | HIS A 220 | 18.194 | 53.243 | 24.711 | 1.00 | 13.99 | 8 | 1794 | CD | ARG A 226 | 28.248 | 66.648 | 30.956 | 1.00 | 9.82 | 6 |
| 1753 | CB | HIS A 220 | 18.055 | 54.802 | 22.293 | 1.00 | 11.69 | 6 | 1795 | NE | ARG A 226 | 29.438 | 67.400 | 31.425 | 1.00 | 9.22 | 7 |
| 1754 | CG | HIS A 220 | 17.630 | 54.760 | 20.840 | 1.00 | 14.69 | 6 | 1796 | CZ | ARG A 226 | 30.251 | 68.074 | 30.592 | 1.00 | 9.27 | 6 |
| 1755 | ND1 | HIS A 220 | 17.984 | 53.694 | 20.064 | 1.00 | 14.71 | 7 | 1797 | NH1 | ARG A 226 | 29.978 | 68.191 | 29.289 | 1.00 | 9.46 | 7 |
| 1756 | CD2 | HIS A 220 | 16.928 | 55.624 | 20.077 | 1.00 | 16.42 | 6 | 1798 | NH2 | ARG A 226 | 31.311 | 68.687 | 31.114 | 1.00 | 10.94 | 7 |
| 1757 | CE1 | HIS A 220 | 17.518 | 53.916 | 18.823 | 1.00 | 16.42 | 6 | 1799 | N | ILE A 227 | 24.590 | 67.940 | 30.262 | 1.00 | 10.46 | 7 |
| 1758 | NE2 | HIS A 220 | 16.855 | 55.077 | 18.794 | 1.00 | 17.85 | 7 | 1800 | CA | ILE A 227 | 24.553 | 68.901 | 29.124 | 1.00 | 7.87 | 6 |
| 1759 | N | GLY A 221 | 16.735 | 54.666 | 25.655 | 1.00 | 11.47 | 7 | 1801 | C | ILE A 227 | 25.807 | 69.751 | 29.238 | 1.00 | 8.86 | 6 |
| 1760 | CA | GLY A 221 | 16.964 | 54.129 | 26.999 | 1.00 | 11.21 | 6 | 1802 | O | ILE A 227 | 26.042 | 70.450 | 30.199 | 1.00 | 11.29 | 8 |
| 1761 | C | GLY A 221 | 17.655 | 55.060 | 27.965 | 1.00 | 13.22 | 6 | 1803 | CB | ILE A 227 | 23.295 | 69.783 | 29.269 | 1.00 | 9.62 | 6 |
| 1762 | O | GLY A 221 | 17.875 | 54.635 | 29.095 | 1.00 | 13.24 | 8 | 1804 | CG1 | ILE A 227 | 22.096 | 68.814 | 29.378 | 1.00 | 10.28 | 6 |
| 1763 | N | ALA A 222 | 18.297 | 56.111 | 27.426 | 1.00 | 12.29 | 7 | 1805 | CG2 | ILE A 227 | 23.196 | 70.601 | 29.964 | 1.00 | 11.21 | 6 |
| 1764 | CA | ALA A 222 | 19.139 | 56.912 | 28.356 | 1.00 | 14.03 | 6 | 1806 | CD1 | ILE A 227 | 20.743 | 69.547 | 29.412 | 1.00 | 15.31 | 6 |
| 1765 | C | ALA A 222 | 18.325 | 57.381 | 29.553 | 1.00 | 13.32 | 6 | 1807 | N | ASP A 228 | 26.544 | 69.672 | 28.125 | 1.00 | 9.30 | 7 |
| 1766 | O | ALA A 222 | 17.138 | 57.794 | 29.459 | 1.00 | 10.61 | 8 | 1808 | CA | ASP A 228 | 27.846 | 70.399 | 28.079 | 1.00 | 9.30 | 6 |
| 1767 | CB | ALA A 222 | 19.700 | 58.136 | 27.618 | 1.00 | 12.95 | 6 | 1809 | C | ASP A 228 | 27.672 | 71.915 | 27.904 | 1.00 | 9.50 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 1810 | O | ASP A 228 | 26.757 | 72.338 | 27.189 | 1.00 | 9.88 | 8 | 1852 | CD1 PHE A 233 | 24.335 | 75.588 | 25.559 | 1.00 | 12.13 | 6 |
| 1811 | CB | ASP A 228 | 28.521 | 69.865 | 26.769 | 1.00 | 9.23 | 6 | 1853 | CD2 PHE A 233 | 22.023 | 76.331 | 25.466 | 1.00 | 11.40 | 6 |
| 1812 | CG | ASP A 228 | 29.904 | 70.442 | 26.587 | 1.00 | 10.24 | 6 | 1854 | CE1 PHE A 233 | 23.982 | 74.503 | 26.347 | 1.00 | 12.18 | 6 |
| 1813 | OD1 | ASP A 228 | 30.725 | 70.228 | 27.505 | 1.00 | 10.28 | 8 | 1855 | CE2 PHE A 233 | 21.642 | 75.219 | 26.237 | 1.00 | 10.50 | 6 |
| 1814 | OD2 | ASP A 228 | 30.208 | 71.128 | 25.574 | 1.00 | 9.89 | 8 | 1856 | CZ PHE A 233 | 22.629 | 74.340 | 26.657 | 1.00 | 11.82 | 6 |
| 1815 | N | ALA A 229 | 28.575 | 72.633 | 28.582 | 1.00 | 8.93 | 7 | 1857 | N ASN A 234 | 22.051 | 80.148 | 25.349 | 1.00 | 12.13 | 7 |
| 1816 | CA | ALA A 229 | 28.745 | 74.068 | 28.257 | 1.00 | 9.72 | 6 | 1858 | CA ASN A 234 | 21.093 | 80.799 | 26.253 | 1.00 | 8.31 | 6 |
| 1817 | C | ALA A 229 | 27.455 | 74.868 | 28.324 | 1.00 | 10.58 | 6 | 1859 | C ASN A 234 | 20.367 | 79.859 | 27.214 | 1.00 | 9.45 | 6 |
| 1818 | O | ALA A 229 | 27.123 | 75.695 | 27.464 | 1.00 | 10.73 | 8 | 1860 | O ASN A 234 | 20.112 | 78.722 | 26.829 | 1.00 | 9.94 | 8 |
| 1819 | CB | ALA A 229 | 29.355 | 74.180 | 26.841 | 1.00 | 9.90 | 6 | 1861 | CB ASN A 234 | 20.132 | 81.662 | 25.369 | 1.00 | 10.71 | 6 |
| 1820 | N | VAL A 230 | 26.729 | 74.708 | 29.487 | 1.00 | 9.05 | 7 | 1862 | CG ASN A 234 | 18.981 | 80.871 | 24.740 | 1.00 | 12.93 | 6 |
| 1821 | CA | VAL A 230 | 25.421 | 75.392 | 29.548 | 1.00 | 9.09 | 6 | 1863 | OD1 ASN A 234 | 18.070 | 80.516 | 25.519 | 1.00 | 12.50 | 8 |
| 1822 | C | VAL A 230 | 25.547 | 76.905 | 29.753 | 1.00 | 10.83 | 6 | 1864 | ND2 ASN A 234 | 18.975 | 80.590 | 23.448 | 1.00 | 10.79 | 7 |
| 1823 | O | VAL A 230 | 24.587 | 77.636 | 29.573 | 1.00 | 12.48 | 8 | 1865 | N SER A 235 | 20.023 | 80.451 | 28.374 | 1.00 | 10.78 | 7 |
| 1824 | CB | VAL A 230 | 24.469 | 74.836 | 30.634 | 1.00 | 10.80 | 6 | 1866 | CA SER A 235 | 19.401 | 79.586 | 29.396 | 1.00 | 8.67 | 6 |
| 1825 | CG1 | VAL A 230 | 24.119 | 73.389 | 30.262 | 1.00 | 9.84 | 6 | 1867 | C SER A 235 | 17.906 | 79.375 | 29.177 | 1.00 | 11.06 | 6 |
| 1826 | CG2 | VAL A 230 | 25.084 | 74.934 | 32.047 | 1.00 | 11.19 | 6 | 1868 | O SER A 235 | 17.399 | 78.402 | 29.759 | 1.00 | 11.56 | 8 |
| 1827 | N | LYS A 231 | 26.753 | 77.312 | 30.189 | 1.00 | 9.10 | 7 | 1869 | CB ASER A 235 | 19.594 | 80.196 | 30.792 | 0.60 | 11.41 | 6 |
| 1828 | CA | LYS A 231 | 26.988 | 78.763 | 30.234 | 1.00 | 7.91 | 6 | 1870 | OG ASER A 235 | 20.974 | 80.269 | 31.098 | 0.60 | 10.81 | 8 |
| 1829 | C | LYS A 231 | 27.304 | 79.391 | 28.883 | 1.00 | 11.01 | 6 | 1869 | CB BSER A 235 | 19.679 | 80.067 | 30.817 | 0.40 | 10.03 | 6 |
| 1830 | O | LYS A 231 | 27.398 | 80.604 | 28.809 | 1.00 | 13.02 | 8 | 1870 | OG BSER A 235 | 19.311 | 81.423 | 30.914 | 0.40 | 7.85 | 8 |
| 1831 | CB | LYS A 231 | 28.173 | 79.043 | 31.209 | 1.00 | 10.48 | 6 | 1871 | N GLY A 236 | 17.301 | 80.140 | 28.312 | 1.00 | 10.81 | 7 |
| 1832 | CG | LYS A 231 | 29.567 | 78.801 | 30.602 | 1.00 | 10.63 | 6 | 1872 | CA GLY A 236 | 15.906 | 79.857 | 27.882 | 1.00 | 11.83 | 5 |
| 1833 | CD | LYS A 231 | 30.599 | 78.817 | 31.758 | 1.00 | 13.70 | 6 | 1873 | C GLY A 236 | 15.821 | 78.448 | 27.289 | 1.00 | 12.34 | 6 |
| 1834 | CE | LYS A 231 | 32.215 | 80.157 | 33.104 | 1.00 | 11.49 | 7 | 1874 | O GLY A 236 | 14.942 | 77.638 | 27.552 | 1.00 | 11.07 | 8 |
| 1835 | NZ | LYS A 231 | 27.364 | 78.589 | 27.814 | 1.00 | 9.37 | 7 | 1875 | N PHE A 237 | 16.742 | 78.158 | 26.370 | 1.00 | 10.75 | 7 |
| 1836 | N | HIS A 232 | 27.744 | 79.081 | 26.480 | 1.00 | 12.72 | 6 | 1876 | CA PHE A 237 | 17.034 | 75.738 | 26.715 | 1.00 | 9.60 | 6 |
| 1837 | CA | HIS A 232 | 26.576 | 79.044 | 25.537 | 1.00 | 12.48 | 6 | 1877 | C PHE A 237 | 16.476 | 74.641 | 26.526 | 1.00 | 10.74 | 8 |
| 1838 | C | HIS A 232 | 26.698 | 79.505 | 24.388 | 1.00 | 9.62 | 8 | 1878 | O PHE A 237 | 17.714 | 76.891 | 24.467 | 1.00 | 12.14 | 6 |
| 1839 | O | HIS A 232 | 28.849 | 78.129 | 25.915 | 1.00 | 9.94 | 6 | 1879 | CB PHE A 237 | 17.642 | 75.595 | 23.691 | 1.00 | 12.02 | 6 |
| 1840 | CB | HIS A 232 | 30.145 | 78.345 | 26.709 | 1.00 | 9.35 | 6 | 1880 | CG PHE A 237 | 16.442 | 75.242 | 23.048 | 1.00 | 12.55 | 6 |
| 1841 | CG | HIS A 232 | 30.780 | 79.598 | 26.674 | 1.00 | 11.03 | 7 | 1881 | CD1 PHE A 237 | 18.751 | 74.740 | 23.659 | 1.00 | 11.64 | 6 |
| 1842 | ND1 | HIS A 232 | 30.803 | 77.530 | 27.554 | 1.00 | 11.85 | 6 | 1882 | CD2 PHE A 237 | 16.367 | 74.046 | 22.358 | 1.00 | 12.60 | 6 |
| 1843 | CD2 | HIS A 232 | 31.838 | 79.483 | 27.513 | 1.00 | 12.22 | 6 | 1883 | CE1 PHE A 237 | 18.634 | 73.533 | 22.952 | 1.00 | 11.39 | 6 |
| 1844 | CE1 | HIS A 232 | 31.882 | 78.243 | 28.049 | 1.00 | 11.68 | 7 | 1884 | CE2 PHE A 237 | 17.468 | 73.200 | 22.301 | 1.00 | 13.43 | 6 |
| 1845 | NE2 | HIS A 232 | 25.342 | 78.757 | 25.941 | 1.00 | 10.57 | 7 | 1885 | CZ PHE A 237 | 17.965 | 75.939 | 27.658 | 1.00 | 10.56 | 7 |
| 1846 | N | PHE A 233 | 23.015 | 79.437 | 25.991 | 1.00 | 9.21 | 6 | 1886 | N SER A 238 | 18.119 | 74.844 | 28.637 | 1.00 | 11.43 | 6 |
| 1847 | CA | PHE A 233 | 23.073 | 79.254 | 27.225 | 1.00 | 11.50 | 8 | 1887 | CA SER A 238 | 16.762 | 74.489 | 29.289 | 1.00 | 10.24 | 6 |
| 1848 | C | PHE A 233 | 23.792 | 77.705 | 24.296 | 1.00 | 9.50 | 6 | 1888 | C SER A 238 | 16.416 | 73.312 | 29.442 | 1.00 | 10.58 | 8 |
| 1849 | O | PHE A 233 | 23.382 | 76.523 | 25.145 | 1.00 | 10.66 | 6 | 1889 | O SER A 238 | 19.069 | 75.303 | 29.776 | 1.00 | 11.86 | 6 |
| 1850 | CB | PHE A 233 | | | | | | | 1890 | CB SER A 238 | 20.432 | 75.070 | 29.404 | 1.00 | 12.16 | 8 |
| 1851 | CG | PHE A 233 | | | | | | | 1891 | OG SER A 238 | | | | | | |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|------------|--------|--------|--------|------|-------|---|
| 1892 | N | LYS A 239 | 16.053 | 75.523 | 29.757 | 1.00 | 10.06 | 7 | 1934 | CD | LYS A 244 | 9.398 | 70.400 | 24.483 | 1.00 | 13.14 | 6 |
| 1893 | CA | LYS A 239 | 14.749 | 75.262 | 30.433 | 1.00 | 10.43 | 6 | 1935 | CE | LYS A 244 | 9.129 | 71.869 | 24.133 | 1.00 | 13.82 | 6 |
| 1894 | C | LYS A 239 | 13.712 | 74.684 | 29.505 | 1.00 | 10.95 | 6 | 1936 | NZ | LYS A 244 | 9.582 | 72.780 | 25.269 | 1.00 | 12.11 | 7 |
| 1895 | O | LYS A 239 | 13.006 | 73.718 | 29.879 | 1.00 | 11.91 | 8 | 1937 | N | LEU A 245 | 12.213 | 67.068 | 27.593 | 1.00 | 11.20 | 7 |
| 1896 | CB | LYS A 239 | 14.259 | 76.598 | 31.123 | 1.00 | 8.56 | 6 | 1938 | CA | LEU A 245 | 12.730 | 65.762 | 28.039 | 1.00 | 11.98 | 6 |
| 1897 | CG | LYS A 239 | 12.889 | 76.329 | 31.861 | 1.00 | 12.08 | 6 | 1939 | C | LEU A 245 | 11.936 | 65.200 | 29.205 | 1.00 | 12.96 | 6 |
| 1898 | CD | LYS A 239 | 12.577 | 77.644 | 32.648 | 1.00 | 11.14 | 6 | 1940 | O | LEU A 245 | 11.665 | 63.996 | 29.219 | 1.00 | 12.16 | 8 |
| 1899 | CE | LYS A 239 | 11.131 | 77.442 | 33.240 | 1.00 | 11.14 | 6 | 1941 | CB | LEU A 245 | 14.221 | 65.961 | 28.461 | 1.00 | 10.88 | 6 |
| 1900 | NZ | LYS A 239 | 10.797 | 78.668 | 34.098 | 1.00 | 10.40 | 7 | 1942 | CG | LEU A 245 | 15.091 | 66.282 | 27.206 | 1.00 | 15.60 | 6 |
| 1901 | N | SER A 240 | 13.600 | 75.153 | 28.279 | 1.00 | 9.61 | 7 | 1943 | CD1 | LEU A 245 | 16.493 | 66.701 | 27.692 | 1.00 | 14.87 | 6 |
| 1902 | CA | SER A 240 | 12.611 | 74.583 | 27.330 | 1.00 | 9.08 | 6 | 1944 | CD2 | LEU A 245 | 15.227 | 65.052 | 26.282 | 1.00 | 19.24 | 6 |
| 1903 | C | SER A 240 | 13.006 | 73.207 | 26.957 | 1.00 | 10.90 | 6 | 1945 | N | TYR A 246 | 11.480 | 66.037 | 30.136 | 1.00 | 11.31 | 7 |
| 1904 | O | SER A 240 | 12.160 | 72.320 | 26.790 | 1.00 | 10.77 | 8 | 1946 | CA | TYR A 246 | 10.676 | 65.529 | 31.258 | 1.00 | 11.13 | 6 |
| 1905 | CB | SER A 240 | 12.560 | 75.572 | 26.136 | 1.00 | 11.38 | 6 | 1947 | C | TYR A 246 | 9.294 | 65.090 | 30.770 | 1.00 | 11.59 | 6 |
| 1906 | OG | SER A 240 | 11.488 | 75.039 | 25.266 | 1.00 | 12.68 | 8 | 1948 | O | TYR A 246 | 8.674 | 64.306 | 31.500 | 1.00 | 13.03 | 8 |
| 1907 | N | LEU A 241 | 14.300 | 72.896 | 26.747 | 1.00 | 10.43 | 7 | 1949 | CB | TYR A 246 | 10.582 | 66.586 | 32.359 | 1.00 | 12.53 | 6 |
| 1908 | CA | LEU A 241 | 14.726 | 71.560 | 26.389 | 1.00 | 10.29 | 6 | 1950 | CG | TYR A 246 | 11.928 | 66.907 | 32.995 | 1.00 | 9.85 | 6 |
| 1909 | C | LEU A 241 | 14.420 | 70.599 | 27.539 | 1.00 | 11.73 | 6 | 1951 | CD1 | TYR A 246 | 12.882 | 65.941 | 33.210 | 1.00 | 11.79 | 6 |
| 1910 | O | LEU A 241 | 13.924 | 69.507 | 27.303 | 1.00 | 11.15 | 8 | 1952 | CD2 | TYR A 246 | 12.163 | 68.228 | 33.408 | 1.00 | 10.52 | 6 |
| 1911 | CB | LEU A 241 | 16.255 | 71.582 | 26.077 | 1.00 | 10.07 | 6 | 1953 | CE1 | TYR A 246 | 14.103 | 66.245 | 33.830 | 1.00 | 11.71 | 6 |
| 1912 | CG | LEU A 241 | 16.816 | 70.170 | 25.829 | 1.00 | 12.71 | 6 | 1954 | CE2 | TYR A 246 | 13.379 | 68.569 | 34.021 | 1.00 | 10.59 | 6 |
| 1913 | CD1 | LEU A 241 | 16.205 | 69.502 | 24.577 | 1.00 | 13.39 | 6 | 1955 | CZ | TYR A 246 | 14.319 | 67.562 | 34.208 | 1.00 | 11.60 | 6 |
| 1914 | CD2 | LEU A 241 | 18.333 | 70.350 | 25.611 | 1.00 | 12.90 | 6 | 1956 | OH | TYR A 246 | 15.536 | 67.856 | 34.816 | 1.00 | 11.49 | 8 |
| 1915 | N | ALA A 242 | 14.710 | 71.055 | 28.778 | 1.00 | 11.25 | 7 | 1957 | N | GLN A 247 | 8.769 | 65.623 | 29.672 | 1.00 | 12.54 | 7 |
| 1916 | CA | ALA A 242 | 14.427 | 70.181 | 29.912 | 1.00 | 10.06 | 6 | 1958 | CA | GLN A 247 | 7.501 | 65.088 | 29.112 | 1.00 | 13.07 | 6 |
| 1917 | C | ALA A 242 | 12.923 | 69.852 | 29.969 | 1.00 | 10.68 | 6 | 1959 | C | GLN A 247 | 7.677 | 63.690 | 28.587 | 1.00 | 13.75 | 6 |
| 1918 | O | ALA A 242 | 12.565 | 68.703 | 30.215 | 1.00 | 10.97 | 8 | 1960 | O | GLN A 247 | 6.712 | 62.875 | 28.651 | 1.00 | 16.16 | 8 |
| 1919 | CB | ALA A 242 | 14.910 | 70.889 | 31.196 | 1.00 | 10.49 | 6 | 1961 | CB | GLN A 247 | 7.016 | 66.001 | 27.940 | 1.00 | 12.33 | 6 |
| 1920 | N | ASP A 243 | 12.062 | 70.870 | 29.712 | 1.00 | 10.40 | 7 | 1962 | CG | GLN A 247 | 6.530 | 67.357 | 28.518 | 1.00 | 13.62 | 6 |
| 1921 | CA | ASP A 243 | 10.609 | 70.595 | 29.694 | 1.00 | 11.54 | 6 | 1963 | CD | GLN A 247 | 6.016 | 68.220 | 27.397 | 1.00 | 16.89 | 6 |
| 1922 | C | ASP A 243 | 10.365 | 69.448 | 28.700 | 1.00 | 12.78 | 6 | 1964 | OE1 | GLN A 247 | 5.355 | 67.699 | 26.462 | 1.00 | 18.89 | 8 |
| 1923 | O | ASP A 243 | 9.636 | 68.474 | 29.006 | 1.00 | 12.31 | 8 | 1965 | NE2 | GLN A 247 | 6.372 | 69.518 | 27.387 | 1.00 | 14.76 | 7 |
| 1924 | CB | ASP A 243 | 9.930 | 71.904 | 29.186 | 1.00 | 11.95 | 6 | 1966 | N | LYS A 248 | 8.881 | 63.349 | 28.162 | 1.00 | 14.17 | 7 |
| 1925 | CG | ASP A 243 | 8.507 | 71.717 | 28.674 | 1.00 | 13.21 | 6 | 1967 | CA | LYS A 248 | 9.163 | 61.979 | 27.702 | 1.00 | 15.18 | 6 |
| 1926 | OD1 | ASP A 243 | 7.668 | 71.113 | 29.422 | 1.00 | 12.98 | 8 | 1968 | C | LYS A 248 | 9.328 | 61.000 | 28.836 | 1.00 | 15.52 | 6 |
| 1927 | OD2 | ASP A 243 | 8.223 | 72.178 | 27.546 | 1.00 | 12.92 | 8 | 1969 | O | LYS A 248 | 8.839 | 59.868 | 28.746 | 1.00 | 16.45 | 8 |
| 1928 | N | LYS A 244 | 10.825 | 69.536 | 27.451 | 1.00 | 10.42 | 7 | 1970 | CB | ALYS A 248 | 10.397 | 61.994 | 26.793 | 0.50 | 13.40 | 6 |
| 1929 | CA | LYS A 244 | 10.523 | 68.449 | 26.484 | 1.00 | 10.94 | 6 | 1971 | CG | ALYS A 248 | 10.116 | 62.793 | 25.528 | 0.50 | 14.14 | 6 |
| 1930 | C | LYS A 244 | 10.997 | 67.097 | 26.998 | 1.00 | 13.31 | 6 | 1972 | CD | ALYS A 248 | 8.958 | 62.165 | 24.749 | 0.50 | 17.69 | 6 |
| 1931 | O | LYS A 244 | 10.349 | 66.061 | 26.763 | 1.00 | 12.24 | 8 | 1973 | CE | ALYS A 248 | 8.449 | 63.068 | 23.657 | 0.50 | 18.41 | 6 |
| 1932 | CB | LYS A 244 | 11.232 | 68.728 | 25.122 | 1.00 | 11.69 | 6 | 1974 | NZ | ALYS A 248 | 7.682 | 62.378 | 22.577 | 0.50 | 25.68 | 7 |
| 1933 | CG | LYS A 244 | 10.924 | 70.142 | 24.580 | 1.00 | 14.16 | 6 | 1970 | CB | BLYS A 248 | 10.414 | 62.030 | 26.816 | 0.50 | 17.60 | 6 |

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|------|-----|------|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 1971 | CG | BLYS | A | 248 | 10.840 | 60.676 | 26.292 | 0.50 | 22.20 | 6 | 2013 | C | LEU | A | 253 | 20.498 | 67.083 | 34.913 | 1.00 | 9.94 | 6 |
| 1972 | CD | BLYS | A | 248 | 11.561 | 60.755 | 24.977 | 0.50 | 29.85 | 6 | 2014 | O | LEU | A | 253 | 20.094 | 67.647 | 35.914 | 1.00 | 11.26 | 8 |
| 1973 | CE | BLYS | A | 248 | 11.495 | 59.497 | 24.150 | 0.50 | 18.09 | 6 | 2015 | CB | LEU | A | 253 | 18.694 | 67.378 | 33.282 | 1.00 | 8.72 | 6 |
| 1974 | NZ | BLYS | A | 248 | 10.779 | 58.367 | 24.885 | 0.50 | 21.86 | 7 | 2016 | CG | LEU | A | 253 | 17.749 | 66.766 | 32.216 | 1.00 | 10.91 | 6 |
| 1975 | N | LYS | A | 249 | 10.131 | 61.400 | 29.830 | 1.00 | 12.97 | 7 | 2017 | CD1 | LEU | A | 253 | 16.881 | 67.891 | 31.562 | 1.00 | 10.35 | 6 |
| 1976 | CA | LYS | A | 249 | 10.424 | 60.442 | 30.917 | 1.00 | 14.04 | 6 | 2018 | CD2 | LEU | A | 253 | 18.508 | 66.051 | 31.089 | 1.00 | 12.13 | 6 |
| 1977 | C | LYS | A | 249 | 10.983 | 61.213 | 32.084 | 1.00 | 11.94 | 6 | 2019 | N | VAL | A | 254 | 21.761 | 67.179 | 34.422 | 1.00 | 11.23 | 7 |
| 1978 | O | LYS | A | 249 | 11.520 | 62.316 | 31.876 | 1.00 | 13.26 | 8 | 2020 | CA | VAL | A | 254 | 22.750 | 68.015 | 35.077 | 1.00 | 11.09 | 6 |
| 1979 | CB | LYS | A | 249 | 11.514 | 59.423 | 30.462 | 1.00 | 15.09 | 6 | 2021 | C | VAL | A | 254 | 23.423 | 68.807 | 33.921 | 1.00 | 10.26 | 6 |
| 1980 | CG | LYS | A | 249 | 11.674 | 58.358 | 31.542 | 1.00 | 15.17 | 6 | 2022 | O | VAL | A | 254 | 23.707 | 68.196 | 32.892 | 1.00 | 10.32 | 8 |
| 1981 | CD | LYS | A | 249 | 12.552 | 57.175 | 31.147 | 1.00 | 23.08 | 6 | 2023 | CB | VAL | A | 254 | 23.722 | 67.184 | 35.947 | 1.00 | 9.61 | 6 |
| 1982 | CE | LYS | A | 249 | 12.451 | 56.111 | 32.249 | 1.00 | 27.89 | 6 | 2024 | CG1 | VAL | A | 254 | 24.552 | 66.161 | 35.161 | 1.00 | 10.99 | 6 |
| 1983 | NZ | LYS | A | 249 | 13.149 | 54.836 | 31.875 | 1.00 | 36.10 | 7 | 2025 | CG2 | VAL | A | 254 | 24.688 | 68.131 | 36.685 | 1.00 | 11.22 | 6 |
| 1984 | N | ASP | A | 250 | 10.870 | 60.678 | 33.288 | 1.00 | 11.41 | 7 | 2026 | N | GLY | A | 255 | 23.762 | 70.047 | 34.194 | 1.00 | 10.96 | 7 |
| 1985 | CA | ASP | A | 250 | 11.406 | 61.336 | 34.494 | 1.00 | 12.04 | 6 | 2027 | CA | GLY | A | 255 | 24.492 | 70.879 | 33.243 | 1.00 | 11.43 | 6 |
| 1986 | C | ASP | A | 250 | 12.918 | 61.011 | 34.626 | 1.00 | 11.51 | 6 | 2028 | C | GLY | A | 255 | 25.877 | 71.193 | 33.731 | 1.00 | 11.23 | 6 |
| 1987 | O | ASP | A | 250 | 13.348 | 60.354 | 35.546 | 1.00 | 13.89 | 8 | 2029 | O | GLY | A | 255 | 26.095 | 71.404 | 34.967 | 1.00 | 10.31 | 8 |
| 1988 | CB | ASP | A | 250 | 10.638 | 60.891 | 35.728 | 1.00 | 11.54 | 6 | 2030 | N | GLU | A | 256 | 26.828 | 71.308 | 32.765 | 1.00 | 10.72 | 7 |
| 1989 | CG | ASP | A | 250 | 10.618 | 59.405 | 36.030 | 1.00 | 15.08 | 8 | 2031 | CA | GLU | A | 256 | 28.159 | 71.786 | 33.187 | 1.00 | 10.84 | 6 |
| 1990 | OD1 | ASP | A | 250 | 10.695 | 58.618 | 35.085 | 1.00 | 15.58 | 8 | 2032 | C | GLU | A | 256 | 28.236 | 73.315 | 33.013 | 1.00 | 11.33 | 6 |
| 1991 | OD2 | ASP | A | 250 | 10.448 | 59.027 | 37.224 | 1.00 | 15.73 | 8 | 2033 | O | GLU | A | 256 | 28.295 | 73.820 | 31.871 | 1.00 | 10.36 | 8 |
| 1992 | N | ILE | A | 251 | 13.644 | 61.541 | 33.607 | 1.00 | 11.19 | 7 | 2034 | CB | GLU | A | 256 | 29.172 | 71.178 | 32.167 | 1.00 | 10.52 | 6 |
| 1993 | CA | ILE | A | 251 | 15.093 | 61.346 | 33.593 | 1.00 | 12.04 | 6 | 2035 | CG | GLU | A | 256 | 30.603 | 71.617 | 32.605 | 1.00 | 10.70 | 6 |
| 1994 | C | ILE | A | 251 | 15.777 | 62.413 | 34.467 | 1.00 | 12.14 | 6 | 2036 | CD | GLU | A | 256 | 31.442 | 72.059 | 31.414 | 1.00 | 11.32 | 6 |
| 1995 | O | ILE | A | 251 | 15.148 | 63.303 | 34.990 | 1.00 | 13.37 | 8 | 2037 | OE1 | GLU | A | 256 | 30.925 | 72.467 | 30.347 | 1.00 | 10.78 | 8 |
| 1996 | CB | ILE | A | 251 | 15.610 | 61.331 | 32.164 | 1.00 | 15.29 | 6 | 2038 | OE2 | GLU | A | 256 | 32.696 | 71.998 | 31.517 | 1.00 | 11.88 | 8 |
| 1997 | CG1 | ILE | A | 251 | 14.988 | 62.477 | 31.361 | 1.00 | 23.77 | 6 | 2039 | N | TRP | A | 257 | 28.173 | 74.038 | 34.120 | 1.00 | 9.79 | 7 |
| 1998 | CG2 | ILE | A | 251 | 15.204 | 60.064 | 31.402 | 1.00 | 16.73 | 6 | 2040 | CA | TRP | A | 257 | 28.409 | 75.480 | 34.158 | 1.00 | 9.57 | 6 |
| 1999 | CD1 | ILE | A | 251 | 15.645 | 63.784 | 31.503 | 1.00 | 25.03 | 6 | 2041 | C | TRP | A | 257 | 29.798 | 75.608 | 34.799 | 1.00 | 10.84 | 6 |
| 2000 | N | PHE | A | 252 | 17.122 | 62.248 | 34.639 | 1.00 | 9.99 | 7 | 2042 | O | TRP | A | 257 | 29.908 | 75.560 | 36.037 | 1.00 | 10.82 | 8 |
| 2001 | CA | PHE | A | 252 | 17.885 | 63.182 | 35.420 | 1.00 | 9.59 | 6 | 2043 | CB | TRP | A | 257 | 27.301 | 76.175 | 34.997 | 1.00 | 9.83 | 6 |
| 2002 | C | PHE | A | 252 | 18.690 | 64.105 | 34.501 | 1.00 | 11.26 | 6 | 2044 | CG | TRP | A | 257 | 27.449 | 77.700 | 34.854 | 1.00 | 8.59 | 6 |
| 2003 | O | PHE | A | 252 | 19.347 | 63.587 | 33.596 | 1.00 | 12.38 | 8 | 2045 | CD1 | TRP | A | 257 | 28.566 | 78.442 | 35.196 | 1.00 | 12.90 | 6 |
| 2004 | CB | PHE | A | 252 | 18.916 | 62.372 | 36.275 | 1.00 | 13.00 | 6 | 2046 | CD2 | TRP | A | 257 | 26.431 | 78.592 | 34.412 | 1.00 | 10.35 | 6 |
| 2005 | CG | PHE | A | 252 | 19.748 | 63.290 | 37.145 | 1.00 | 11.27 | 6 | 2047 | NE1 | TRP | A | 257 | 28.295 | 79.753 | 34.937 | 1.00 | 12.55 | 7 |
| 2006 | CD1 | PHE | A | 252 | 19.182 | 63.951 | 38.241 | 1.00 | 12.24 | 6 | 2048 | CE2 | TRP | A | 257 | 27.020 | 79.891 | 34.459 | 1.00 | 12.29 | 6 |
| 2007 | CD2 | PHE | A | 252 | 21.094 | 63.494 | 36.838 | 1.00 | 12.52 | 6 | 2049 | CE3 | TRP | A | 257 | 25.124 | 78.425 | 33.946 | 1.00 | 13.94 | 6 |
| 2008 | CE1 | PHE | A | 252 | 19.907 | 64.802 | 39.029 | 1.00 | 11.05 | 6 | 2050 | CZ2 | TRP | A | 257 | 26.317 | 81.041 | 34.055 | 1.00 | 10.73 | 6 |
| 2009 | CE2 | PHE | A | 252 | 21.843 | 64.327 | 37.664 | 1.00 | 11.26 | 6 | 2051 | CZ3 | TRP | A | 257 | 24.385 | 79.544 | 33.527 | 1.00 | 13.32 | 6 |
| 2010 | CZ | PHE | A | 252 | 21.263 | 65.031 | 38.750 | 1.00 | 10.84 | 6 | 2052 | CH2 | TRP | A | 257 | 25.026 | 80.793 | 33.599 | 1.00 | 11.64 | 6 |
| 2011 | N | LEU | A | 253 | 18.740 | 65.389 | 34.772 | 1.00 | 12.09 | 7 | 2053 | N | TYR | A | 258 | 30.831 | 75.725 | 33.986 | 1.00 | 11.79 | 7 |
| 2012 | CA | LEU | A | 253 | 19.592 | 66.278 | 33.936 | 1.00 | 9.30 | 6 | 2054 | CA | TYR | A | 258 | 32.211 | 75.619 | 34.524 | 1.00 | 11.80 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2055 | C | TYR A 258 | 32.527 | 76.859 | 35.355 | 1.00 | 12.06 | 6 | 2097 | CA | THR A 264 | 32.579 | 85.990 | 41.270 | 1.00 | 15.29 | 6 |
| 2056 | O | TYR A 258 | 32.370 | 77.988 | 34.869 | 1.00 | 13.57 | 8 | 2098 | C | THR A 264 | 31.378 | 86.647 | 40.599 | 1.00 | 14.14 | 6 |
| 2057 | CB | TYR A 258 | 33.189 | 75.508 | 33.335 | 1.00 | 11.31 | 6 | 2099 | O | THR A 264 | 30.225 | 86.490 | 41.019 | 1.00 | 15.14 | 8 |
| 2058 | CG | TYR A 258 | 34.562 | 74.978 | 33.723 | 1.00 | 11.97 | 6 | 2100 | CB | THR A 264 | 33.154 | 84.890 | 40.377 | 1.00 | 17.00 | 6 |
| 2059 | CD1 | TYR A 258 | 35.452 | 75.687 | 34.524 | 1.00 | 13.71 | 6 | 2101 | OG1 | THR A 264 | 32.185 | 83.864 | 40.214 | 1.00 | 17.20 | 8 |
| 2060 | CD2 | TYR A 258 | 34.932 | 73.734 | 33.234 | 1.00 | 11.78 | 6 | 2102 | CG2 | THR A 264 | 34.455 | 84.302 | 40.998 | 1.00 | 18.53 | 6 |
| 2061 | CE1 | TYR A 258 | 36.707 | 75.160 | 34.859 | 1.00 | 15.77 | 6 | 2103 | N | ALA A 265 | 31.684 | 87.407 | 39.536 | 1.00 | 14.47 | 7 |
| 2062 | CE2 | TYR A 258 | 36.179 | 73.226 | 33.564 | 1.00 | 13.38 | 6 | 2104 | CA | ALA A 265 | 30.579 | 88.206 | 38.957 | 1.00 | 16.68 | 6 |
| 2063 | CZ | TYR A 258 | 37.037 | 73.908 | 34.376 | 1.00 | 16.44 | 6 | 2105 | C | ALA A 265 | 29.455 | 87.387 | 38.348 | 1.00 | 14.50 | 6 |
| 2064 | OH | TYR A 258 | 38.277 | 73.304 | 34.631 | 1.00 | 20.59 | 8 | 2106 | O | ALA A 265 | 28.315 | 87.921 | 38.116 | 1.00 | 15.71 | 8 |
| 2065 | N | GLY A 259 | 33.030 | 76.605 | 36.550 | 1.00 | 9.86 | 7 | 2107 | CB | ALA A 265 | 31.153 | 89.034 | 37.793 | 1.00 | 18.93 | 6 |
| 2066 | CA | GLY A 259 | 33.584 | 77.705 | 37.361 | 1.00 | 12.24 | 6 | 2108 | N | ASN A 266 | 29.808 | 86.186 | 37.837 | 1.00 | 11.26 | 7 |
| 2067 | C | GLY A 259 | 32.510 | 78.690 | 37.891 | 1.00 | 11.55 | 6 | 2109 | CA | ASN A 266 | 28.739 | 85.402 | 37.199 | 1.00 | 12.93 | 6 |
| 2068 | O | GLY A 259 | 31.417 | 78.276 | 38.227 | 1.00 | 12.61 | 8 | 2110 | C | ASN A 266 | 28.140 | 84.338 | 38.110 | 1.00 | 13.52 | 6 |
| 2069 | N | ASP A 260 | 32.921 | 79.963 | 37.891 | 1.00 | 11.45 | 7 | 2111 | O | ASN A 266 | 27.364 | 83.484 | 37.632 | 1.00 | 11.82 | 8 |
| 2070 | CA | ASP A 260 | 32.064 | 81.004 | 38.486 | 1.00 | 10.59 | 6 | 2112 | CB | ASN A 266 | 29.289 | 84.792 | 35.855 | 1.00 | 15.03 | 6 |
| 2071 | C | ASP A 260 | 31.718 | 80.614 | 39.947 | 1.00 | 12.08 | 6 | 2113 | CG | ASN A 266 | 29.632 | 85.944 | 34.889 | 1.00 | 15.26 | 6 |
| 2072 | O | ASP A 260 | 30.554 | 80.528 | 40.317 | 1.00 | 11.34 | 8 | 2114 | OD1 | ASN A 266 | 28.938 | 86.955 | 34.822 | 1.00 | 13.24 | 8 |
| 2073 | CB | ASP A 260 | 30.792 | 81.286 | 37.665 | 1.00 | 13.01 | 6 | 2115 | ND2 | ASN A 266 | 30.698 | 85.797 | 34.146 | 1.00 | 14.64 | 7 |
| 2074 | CA | ASP A 260 | 31.160 | 81.807 | 36.269 | 1.00 | 16.43 | 6 | 2116 | N | HIS A 267 | 28.621 | 84.306 | 39.353 | 1.00 | 12.23 | 7 |
| 2075 | OD1 | ASP A 260 | 32.136 | 82.593 | 36.148 | 1.00 | 13.58 | 8 | 2117 | CA | HIS A 267 | 28.106 | 83.276 | 40.271 | 1.00 | 13.10 | 6 |
| 2076 | OD2 | ASP A 260 | 30.486 | 81.502 | 35.274 | 1.00 | 14.47 | 8 | 2118 | C | HIS A 267 | 26.596 | 83.276 | 40.469 | 1.00 | 13.44 | 6 |
| 2077 | N | ASP A 261 | 32.812 | 80.528 | 40.708 | 1.00 | 10.89 | 7 | 2119 | O | HIS A 267 | 25.999 | 82.182 | 40.399 | 1.00 | 12.11 | 8 |
| 2078 | CA | ASP A 261 | 32.709 | 80.239 | 42.158 | 1.00 | 13.96 | 6 | 2120 | CB | HIS A 267 | 28.852 | 83.439 | 41.616 | 1.00 | 10.82 | 6 |
| 2079 | C | ASP A 261 | 32.059 | 81.369 | 42.936 | 1.00 | 12.00 | 6 | 2121 | CG | HIS A 267 | 28.469 | 82.306 | 42.563 | 1.00 | 12.37 | 6 |
| 2080 | O | ASP A 261 | 31.920 | 82.528 | 42.502 | 1.00 | 13.08 | 8 | 2122 | ND1 | HIS A 267 | 28.877 | 81.020 | 42.410 | 1.00 | 11.65 | 7 |
| 2081 | CB | ASP A 261 | 34.125 | 79.875 | 42.610 | 1.00 | 17.34 | 6 | 2123 | CD2 | HIS A 267 | 27.637 | 82.360 | 43.640 | 1.00 | 15.29 | 6 |
| 2082 | CG | ASP A 261 | 34.615 | 78.518 | 42.074 | 1.00 | 18.47 | 6 | 2124 | CE1 | HIS A 267 | 28.355 | 80.278 | 43.375 | 1.00 | 12.97 | 6 |
| 2083 | OD1 | ASP A 261 | 33.990 | 77.881 | 41.181 | 1.00 | 22.23 | 8 | 2125 | NE2 | HIS A 267 | 27.608 | 81.080 | 44.153 | 1.00 | 11.63 | 7 |
| 2084 | OD2 | ASP A 261 | 35.642 | 78.035 | 42.569 | 1.00 | 20.46 | 8 | 2126 | N | LEU A 268 | 26.001 | 84.430 | 40.726 | 1.00 | 10.81 | 7 |
| 2085 | N | PRO A 262 | 31.751 | 81.124 | 44.230 | 1.00 | 11.36 | 7 | 2127 | CA | LEU A 268 | 24.548 | 84.455 | 40.988 | 1.00 | 13.40 | 6 |
| 2086 | CA | PRO A 262 | 31.155 | 82.197 | 45.033 | 1.00 | 13.50 | 6 | 2128 | C | LEU A 268 | 23.766 | 83.997 | 39.768 | 1.00 | 11.02 | 6 |
| 2087 | C | PRO A 262 | 32.085 | 83.428 | 45.042 | 1.00 | 15.27 | 6 | 2129 | O | LEU A 268 | 22.745 | 83.268 | 39.957 | 1.00 | 12.74 | 8 |
| 2088 | O | PRO A 262 | 33.325 | 83.254 | 45.078 | 1.00 | 17.80 | 8 | 2130 | CB | LEU A 268 | 24.169 | 85.889 | 41.374 | 1.00 | 14.95 | 6 |
| 2089 | CB | PRO A 262 | 30.973 | 81.583 | 46.445 | 1.00 | 14.74 | 6 | 2131 | CG | LEU A 268 | 22.599 | 86.052 | 41.471 | 1.00 | 19.99 | 6 |
| 2090 | CG | PRO A 262 | 30.818 | 80.086 | 46.071 | 1.00 | 13.76 | 6 | 2132 | CD1 | LEU A 268 | 22.040 | 85.151 | 42.563 | 1.00 | 24.25 | 6 |
| 2091 | CD | PRO A 262 | 31.873 | 79.856 | 44.938 | 1.00 | 11.66 | 6 | 2133 | CD2 | LEU A 268 | 22.298 | 87.536 | 41.677 | 1.00 | 25.18 | 6 |
| 2092 | N | GLY A 263 | 31.385 | 84.560 | 45.069 | 1.00 | 20.11 | 7 | 2134 | N | GLU A 269 | 24.210 | 84.274 | 38.549 | 1.00 | 11.51 | 7 |
| 2093 | CA | GLY A 263 | 32.178 | 85.810 | 45.091 | 1.00 | 20.82 | 6 | 2135 | CA | GLU A 269 | 23.495 | 83.760 | 37.381 | 1.00 | 11.81 | 6 |
| 2094 | C | GLY A 263 | 32.444 | 86.343 | 43.693 | 1.00 | 22.93 | 6 | 2136 | C | GLU A 269 | 23.525 | 82.221 | 37.386 | 1.00 | 10.11 | 6 |
| 2095 | O | GLY A 263 | 33.030 | 87.433 | 43.565 | 1.00 | 26.12 | 8 | 2137 | O | GLU A 269 | 22.512 | 81.596 | 37.067 | 1.00 | 11.07 | 8 |
| 2096 | N | THR A 264 | 32.204 | 85.581 | 42.640 | 1.00 | 16.30 | 7 | 2138 | CB | GLU A 269 | 24.190 | 84.360 | 36.122 | 1.00 | 13.26 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2139 | CG | GIU A 269 | 23.490 | 83.803 | 34.867 | 1.00 | 11.45 | 6 | 2181 | OH | TYR A 273 | 21.365 | 74.258 | 31.956 | 1.00 | 11.35 | 8 |
| 2140 | CD | GIU A 269 | 24.122 | 84.417 | 33.582 | 1.00 | 13.11 | 6 | 2182 | N | ALA A 274 | 20.678 | 77.001 | 38.308 | 1.00 | 10.68 | 7 |
| 2141 | OE1 | GIU A 269 | 24.906 | 85.369 | 33.643 | 1.00 | 12.92 | 8 | 2183 | CA | ALA A 274 | 20.449 | 75.597 | 39.008 | 1.00 | 10.66 | 6 |
| 2142 | OE2 | GIU A 269 | 23.720 | 83.906 | 32.525 | 1.00 | 12.17 | 8 | 2184 | C | ALA A 274 | 19.062 | 75.725 | 39.677 | 1.00 | 10.79 | 6 |
| 2143 | N | LVS A 270 | 24.678 | 81.608 | 37.720 | 1.00 | 9.00 | 7 | 2185 | O | ALA A 274 | 18.478 | 74.649 | 39.796 | 1.00 | 11.53 | 8 |
| 2144 | CA | LVS A 270 | 24.754 | 80.156 | 37.787 | 1.00 | 9.72 | 6 | 2186 | CB | ALA A 274 | 21.539 | 75.560 | 40.092 | 1.00 | 12.82 | 6 |
| 2145 | C | LVS A 270 | 23.806 | 79.578 | 38.862 | 1.00 | 10.98 | 6 | 2187 | N | ASN A 275 | 18.692 | 76.887 | 40.217 | 1.00 | 11.15 | 7 |
| 2146 | O | LVS A 270 | 23.079 | 78.613 | 38.609 | 1.00 | 10.64 | 8 | 2188 | CA | ASN A 275 | 17.443 | 76.882 | 40.998 | 1.00 | 11.26 | 6 |
| 2147 | CB | LVS A 270 | 26.221 | 79.709 | 38.063 | 1.00 | 10.49 | 6 | 2189 | C | ASN A 275 | 16.199 | 77.051 | 40.131 | 1.00 | 10.88 | 6 |
| 2148 | CG | LVS A 270 | 26.259 | 78.174 | 38.299 | 1.00 | 10.05 | 6 | 2190 | O | ASN A 275 | 15.082 | 76.705 | 40.606 | 1.00 | 11.83 | 8 |
| 2149 | CD | LVS A 270 | 27.725 | 77.682 | 38.502 | 1.00 | 8.77 | 6 | 2191 | CB | ASN A 275 | 17.490 | 78.056 | 42.004 | 1.00 | 11.31 | 6 |
| 2150 | CE | LVS A 270 | 28.236 | 78.181 | 39.869 | 1.00 | 9.57 | 6 | 2192 | CG | ASN A 275 | 18.495 | 77.768 | 43.107 | 1.00 | 11.97 | 6 |
| 2151 | NZ | LVS A 270 | 29.600 | 77.515 | 40.161 | 1.00 | 11.56 | 7 | 2193 | OD1 | ASN A 275 | 18.987 | 76.561 | 43.214 | 1.00 | 12.55 | 8 |
| 2152 | N | VAL A 271 | 23.765 | 80.218 | 40.038 | 1.00 | 11.90 | 7 | 2194 | ND2 | ASN A 275 | 18.759 | 78.816 | 43.934 | 1.00 | 12.55 | 7 |
| 2153 | CA | VAL A 271 | 22.847 | 79.712 | 41.105 | 1.00 | 10.97 | 6 | 2195 | N | ASN A 276 | 16.322 | 77.453 | 38.842 | 1.00 | 11.20 | 7 |
| 2154 | C | VAL A 271 | 21.392 | 79.835 | 40.608 | 1.00 | 10.81 | 6 | 2196 | CA | ASN A 276 | 15.129 | 77.705 | 38.045 | 1.00 | 12.25 | 6 |
| 2155 | O | VAL A 271 | 20.583 | 78.951 | 40.827 | 1.00 | 11.67 | 8 | 2197 | C | ASN A 276 | 15.023 | 76.992 | 36.720 | 1.00 | 14.18 | 6 |
| 2156 | CB | VAL A 271 | 23.044 | 80.608 | 42.346 | 1.00 | 13.53 | 6 | 2198 | O | ASN A 276 | 13.932 | 76.920 | 36.165 | 1.00 | 11.89 | 8 |
| 2157 | CG1 | VAL A 271 | 22.016 | 80.248 | 43.435 | 1.00 | 12.11 | 6 | 2199 | CB | ASN A 276 | 15.134 | 79.197 | 37.632 | 1.00 | 9.94 | 6 |
| 2158 | CG2 | VAL A 271 | 24.455 | 80.307 | 42.888 | 1.00 | 12.46 | 6 | 2200 | CG | ASN A 276 | 14.629 | 80.023 | 38.806 | 1.00 | 14.75 | 6 |
| 2159 | N | ARG A 272 | 21.064 | 80.978 | 39.983 | 1.00 | 11.20 | 7 | 2201 | OD1 | ASN A 276 | 13.365 | 80.089 | 38.826 | 1.00 | 16.83 | 8 |
| 2160 | CA | ARG A 272 | 19.668 | 81.127 | 39.458 | 1.00 | 11.53 | 6 | 2202 | ND2 | ASN A 276 | 15.551 | 80.529 | 39.612 | 1.00 | 16.12 | 7 |
| 2161 | C | ARG A 272 | 19.328 | 80.041 | 38.439 | 1.00 | 10.29 | 6 | 2203 | N | SER A 277 | 16.151 | 76.504 | 36.173 | 1.00 | 10.52 | 7 |
| 2162 | O | ARG A 272 | 18.208 | 79.506 | 38.389 | 1.00 | 11.34 | 8 | 2204 | CA | SER A 277 | 16.064 | 75.974 | 34.811 | 1.00 | 11.82 | 6 |
| 2163 | CB | ARG A 272 | 19.462 | 82.540 | 38.859 | 1.00 | 9.74 | 6 | 2205 | C | SER A 277 | 15.497 | 74.585 | 34.678 | 1.00 | 11.16 | 6 |
| 2164 | CG | ARG A 272 | 19.220 | 83.552 | 40.027 | 1.00 | 11.97 | 6 | 2206 | O | SER A 277 | 15.204 | 74.178 | 33.545 | 1.00 | 12.16 | 8 |
| 2165 | CD | ARG A 272 | 19.405 | 85.000 | 39.483 | 1.00 | 10.96 | 6 | 2207 | CB | SER A 277 | 17.502 | 75.911 | 34.204 | 1.00 | 11.66 | 6 |
| 2166 | NE | ARG A 272 | 18.600 | 85.394 | 38.306 | 1.00 | 12.10 | 7 | 2208 | OG | SER A 277 | 18.257 | 74.877 | 34.872 | 1.00 | 12.14 | 8 |
| 2167 | CZ | ARG A 272 | 17.297 | 85.759 | 38.377 | 1.00 | 14.61 | 6 | 2209 | N | GLY A 278 | 15.371 | 73.851 | 35.795 | 1.00 | 11.36 | 7 |
| 2168 | NH1 | ARG A 272 | 16.541 | 85.765 | 39.493 | 1.00 | 12.14 | 7 | 2210 | CA | GLY A 278 | 15.051 | 72.411 | 35.697 | 1.00 | 11.40 | 6 |
| 2169 | NH2 | ARG A 272 | 16.734 | 86.132 | 37.232 | 1.00 | 12.07 | 7 | 2211 | C | GLY A 278 | 16.263 | 71.565 | 35.375 | 1.00 | 11.97 | 6 |
| 2170 | N | TYR A 273 | 20.329 | 79.790 | 37.553 | 1.00 | 10.33 | 7 | 2212 | O | GLY A 278 | 16.115 | 70.348 | 35.279 | 1.00 | 13.61 | 8 |
| 2171 | CA | TYR A 273 | 20.116 | 78.669 | 36.589 | 1.00 | 11.57 | 6 | 2213 | N | VAL A 279 | 17.442 | 72.180 | 35.342 | 1.00 | 12.14 | 7 |
| 2172 | C | TYR A 273 | 19.882 | 77.355 | 37.328 | 1.00 | 9.14 | 6 | 2214 | CA | VAL A 279 | 18.673 | 71.427 | 35.090 | 1.00 | 10.48 | 6 |
| 2173 | O | TYR A 273 | 18.931 | 76.590 | 36.993 | 1.00 | 12.29 | 8 | 2215 | C | VAL A 279 | 19.552 | 71.645 | 36.348 | 1.00 | 11.31 | 6 |
| 2174 | CB | TYR A 273 | 21.415 | 78.569 | 35.742 | 1.00 | 9.07 | 6 | 2216 | O | VAL A 279 | 19.814 | 72.782 | 36.732 | 1.00 | 12.60 | 8 |
| 2175 | CG | TYR A 273 | 21.388 | 77.445 | 34.693 | 1.00 | 8.78 | 6 | 2217 | CB | VAL A 279 | 19.362 | 71.989 | 33.830 | 1.00 | 11.56 | 6 |
| 2176 | CD1 | TYR A 273 | 21.708 | 76.144 | 35.110 | 1.00 | 11.52 | 6 | 2218 | CG1 | VAL A 279 | 20.628 | 71.191 | 33.543 | 1.00 | 10.87 | 6 |
| 2177 | CD2 | TYR A 273 | 21.054 | 77.630 | 33.363 | 1.00 | 9.55 | 6 | 2219 | CG2 | VAL A 279 | 18.429 | 71.824 | 32.592 | 1.00 | 13.38 | 6 |
| 2178 | CE1 | TYR A 273 | 21.663 | 75.071 | 34.218 | 1.00 | 9.62 | 6 | 2220 | N | ASN A 280 | 20.053 | 70.556 | 36.919 | 1.00 | 10.03 | 7 |
| 2179 | CE2 | TYR A 273 | 21.087 | 76.577 | 32.482 | 1.00 | 8.45 | 6 | 2221 | CA | ASN A 280 | 20.918 | 70.714 | 38.122 | 1.00 | 10.49 | 6 |
| 2180 | CZ | TYR A 273 | 21.366 | 75.301 | 32.885 | 1.00 | 10.47 | 6 | 2222 | C | ASN A 280 | 22.294 | 71.095 | 37.572 | 1.00 | 13.05 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2223 | O | ASN A 280 | 22.506 | 71.116 | 36.365 | 1.00 | 12.57 | 8 | 2265 | O | ASP A 285 | 33.806 | 75.092 | 45.468 | 1.00 | 11.00 | 8 |
| 2224 | CB | ASN A 280 | 20.968 | 69.368 | 38.864 | 1.00 | 11.26 | 6 | 2266 | CB | ASP A 285 | 30.773 | 76.068 | 44.545 | 1.00 | 9.55 | 6 |
| 2225 | CG | ASN A 280 | 19.492 | 69.056 | 39.263 | 1.00 | 9.85 | 6 | 2267 | CG | ASP A 285 | 29.979 | 77.042 | 43.692 | 1.00 | 10.92 | 6 |
| 2226 | OD1 | ASN A 280 | 18.839 | 69.805 | 39.990 | 1.00 | 10.91 | 8 | 2268 | OD1 | ASP A 285 | 30.499 | 77.631 | 42.710 | 1.00 | 12.04 | 8 |
| 2227 | ND2 | ASN A 280 | 18.974 | 67.913 | 38.787 | 1.00 | 10.65 | 7 | 2269 | OD2 | ASP A 285 | 28.773 | 77.214 | 44.043 | 1.00 | 12.59 | 8 |
| 2228 | N | VAL A 281 | 23.262 | 71.312 | 38.492 | 1.00 | 11.45 | 7 | 2270 | N | LEU A 286 | 32.248 | 73.464 | 45.128 | 1.00 | 10.30 | 7 |
| 2229 | CA | VAL A 281 | 24.622 | 71.621 | 37.977 | 1.00 | 9.71 | 6 | 2271 | CA | LEU A 286 | 32.959 | 72.569 | 46.061 | 1.00 | 9.08 | 6 |
| 2230 | C | VAL A 281 | 25.671 | 70.782 | 38.660 | 1.00 | 11.24 | 6 | 2272 | C | LEU A 286 | 34.219 | 71.940 | 45.505 | 1.00 | 9.26 | 6 |
| 2231 | O | VAL A 281 | 25.581 | 70.318 | 39.799 | 1.00 | 11.15 | 8 | 2273 | O | LEU A 286 | 35.179 | 71.757 | 46.238 | 1.00 | 11.04 | 8 |
| 2232 | CB | VAL A 281 | 25.013 | 73.104 | 38.187 | 1.00 | 9.82 | 6 | 2274 | CB | LEU A 286 | 31.968 | 71.419 | 46.481 | 1.00 | 9.12 | 6 |
| 2233 | CG1 | VAL A 281 | 24.019 | 74.024 | 37.397 | 1.00 | 10.47 | 6 | 2275 | CG | LEU A 286 | 32.367 | 70.697 | 47.790 | 1.00 | 10.68 | 6 |
| 2234 | CG2 | VAL A 281 | 25.038 | 73.569 | 39.638 | 1.00 | 11.52 | 6 | 2276 | CD1 | LEU A 286 | 32.357 | 71.580 | 49.023 | 1.00 | 15.93 | 6 |
| 2235 | N | LEU A 282 | 26.786 | 70.675 | 37.904 | 1.00 | 9.31 | 7 | 2277 | CD2 | LEU A 286 | 31.384 | 69.510 | 47.999 | 1.00 | 13.68 | 6 |
| 2236 | CA | LEU A 282 | 28.031 | 70.087 | 38.460 | 1.00 | 10.27 | 6 | 2278 | N | ASN A 287 | 34.226 | 71.683 | 44.168 | 1.00 | 9.32 | 7 |
| 2237 | C | LEU A 282 | 28.631 | 71.063 | 39.476 | 1.00 | 11.17 | 6 | 2279 | CA | ASN A 287 | 35.441 | 71.091 | 43.586 | 1.00 | 10.65 | 6 |
| 2238 | O | LEU A 282 | 28.577 | 72.295 | 39.298 | 1.00 | 12.65 | 8 | 2280 | C | ASN A 287 | 36.687 | 71.937 | 43.872 | 1.00 | 9.75 | 6 |
| 2239 | CB | LEU A 282 | 29.022 | 69.883 | 37.283 | 1.00 | 10.13 | 6 | 2281 | O | ASN A 287 | 37.751 | 71.401 | 44.184 | 1.00 | 10.35 | 8 |
| 2240 | CG | LEU A 282 | 28.650 | 68.558 | 36.538 | 1.00 | 11.97 | 6 | 2282 | CB | ASN A 287 | 35.269 | 71.000 | 42.039 | 1.00 | 8.74 | 6 |
| 2241 | CD1 | LEU A 282 | 29.159 | 68.726 | 35.102 | 1.00 | 16.51 | 6 | 2283 | CG | ASN A 287 | 36.571 | 70.507 | 41.392 | 1.00 | 11.79 | 6 |
| 2242 | CD2 | LEU A 282 | 29.314 | 67.351 | 37.196 | 1.00 | 12.93 | 6 | 2284 | OD1 | ASN A 287 | 37.171 | 71.318 | 40.654 | 1.00 | 11.65 | 8 |
| 2243 | N | ASP A 283 | 29.128 | 70.458 | 40.581 | 1.00 | 9.33 | 7 | 2285 | ND2 | ASN A 287 | 36.866 | 69.245 | 41.597 | 1.00 | 9.92 | 7 |
| 2244 | CA | ASP A 283 | 29.503 | 71.304 | 41.764 | 1.00 | 11.76 | 6 | 2286 | N | THR A 288 | 36.588 | 73.275 | 43.719 | 1.00 | 9.52 | 7 |
| 2245 | C | ASP A 283 | 30.935 | 71.778 | 41.696 | 1.00 | 11.31 | 6 | 2287 | CA | THR A 288 | 37.769 | 74.106 | 43.907 | 1.00 | 11.58 | 6 |
| 2246 | O | ASP A 283 | 31.877 | 71.275 | 42.316 | 1.00 | 11.22 | 8 | 2288 | C | THR A 288 | 38.367 | 73.906 | 45.292 | 1.00 | 10.74 | 6 |
| 2247 | CB | ASP A 283 | 29.212 | 70.451 | 43.014 | 1.00 | 8.73 | 6 | 2289 | O | THR A 288 | 39.593 | 73.741 | 45.486 | 1.00 | 13.25 | 8 |
| 2248 | CG | ASP A 283 | 29.282 | 71.343 | 44.271 | 1.00 | 11.60 | 6 | 2290 | CB | THR A 288 | 37.365 | 75.596 | 43.745 | 1.00 | 15.82 | 6 |
| 2249 | OD1 | ASP A 283 | 29.655 | 72.526 | 44.259 | 1.00 | 10.06 | 8 | 2291 | OG1 | THR A 288 | 36.906 | 75.753 | 42.397 | 1.00 | 16.55 | 8 |
| 2250 | OD2 | ASP A 283 | 28.866 | 70.758 | 45.290 | 1.00 | 11.95 | 8 | 2292 | CG2 | THR A 288 | 38.641 | 76.459 | 43.984 | 1.00 | 14.43 | 6 |
| 2251 | N | PHE A 284 | 31.108 | 72.815 | 40.834 | 1.00 | 10.41 | 7 | 2293 | N | VAL A 289 | 37.440 | 73.847 | 46.268 | 1.00 | 8.64 | 7 |
| 2252 | CA | PHE A 284 | 32.439 | 73.424 | 40.731 | 1.00 | 10.33 | 6 | 2294 | CA | VAL A 289 | 37.915 | 73.732 | 47.655 | 1.00 | 8.82 | 6 |
| 2253 | C | PHE A 284 | 32.746 | 74.271 | 41.966 | 1.00 | 11.21 | 6 | 2295 | C | VAL A 289 | 38.401 | 72.341 | 47.985 | 1.00 | 11.04 | 6 |
| 2254 | O | PHE A 284 | 33.941 | 74.331 | 42.313 | 1.00 | 12.52 | 8 | 2296 | O | VAL A 289 | 39.438 | 72.184 | 48.642 | 1.00 | 11.67 | 8 |
| 2255 | CB | PHE A 284 | 32.509 | 74.409 | 39.517 | 1.00 | 10.51 | 6 | 2297 | CB | VAL A 289 | 36.780 | 74.237 | 48.605 | 1.00 | 11.02 | 6 |
| 2256 | CG | PHE A 284 | 32.750 | 73.575 | 38.227 | 1.00 | 10.01 | 6 | 2298 | CG1 | VAL A 289 | 37.297 | 74.258 | 50.051 | 1.00 | 10.38 | 6 |
| 2257 | CD1 | PHE A 284 | 31.725 | 72.991 | 37.520 | 1.00 | 11.07 | 6 | 2299 | CG2 | VAL A 289 | 36.323 | 75.632 | 48.191 | 1.00 | 11.61 | 6 |
| 2258 | CD2 | PHE A 284 | 34.073 | 73.416 | 37.765 | 1.00 | 11.57 | 6 | 2300 | N | ILE A 290 | 37.764 | 71.287 | 47.430 | 1.00 | 9.86 | 7 |
| 2259 | CE1 | PHE A 284 | 31.925 | 72.232 | 36.386 | 1.00 | 12.29 | 6 | 2301 | CA | ILE A 290 | 38.262 | 69.911 | 47.642 | 1.00 | 8.30 | 6 |
| 2260 | CE2 | PHE A 284 | 34.292 | 72.665 | 36.596 | 1.00 | 11.45 | 6 | 2302 | C | ILE A 290 | 39.715 | 69.830 | 47.144 | 1.00 | 12.22 | 6 |
| 2261 | CZ | PHE A 284 | 33.234 | 72.085 | 35.903 | 1.00 | 9.72 | 6 | 2303 | O | ILE A 290 | 40.554 | 69.251 | 47.806 | 1.00 | 10.89 | 8 |
| 2262 | N | ASP A 285 | 31.729 | 74.753 | 42.687 | 1.00 | 9.13 | 7 | 2304 | CB | ILE A 290 | 37.342 | 68.979 | 46.851 | 1.00 | 9.93 | 6 |
| 2263 | CA | ASP A 285 | 32.061 | 75.575 | 43.882 | 1.00 | 10.61 | 6 | 2305 | CG1 | ILE A 290 | 36.004 | 68.833 | 47.591 | 1.00 | 11.46 | 6 |
| 2264 | C | ASP A 285 | 32.799 | 74.670 | 44.885 | 1.00 | 10.95 | 6 | 2306 | CG2 | ILE A 290 | 38.025 | 67.579 | 46.690 | 1.00 | 11.35 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2307 | CD1 | ILE A 290 | 34.964 | 68.108 | 46.700 | 1.00 | 11.71 | 6 | 2349 | N | THR A 296 | 46.271 | 70.499 | 46.990 | 1.00 | 10.00 | 7 |
| 2308 | N | ARG A 291 | 39.969 | 70.386 | 45.940 | 1.00 | 11.21 | 7 | 2350 | CA | THR A 296 | 47.441 | 71.394 | 47.123 | 1.00 | 11.19 | 6 |
| 2309 | CA | ARG A 291 | 41.352 | 70.246 | 45.455 | 1.00 | 10.67 | 6 | 2351 | C | THR A 296 | 47.675 | 71.894 | 48.549 | 1.00 | 13.50 | 6 |
| 2310 | C | ARG A 291 | 42.343 | 71.071 | 46.293 | 1.00 | 9.59 | 6 | 2352 | O | THR A 296 | 48.755 | 72.436 | 48.874 | 1.00 | 12.22 | 8 |
| 2311 | O | ARG A 291 | 43.481 | 70.627 | 46.380 | 1.00 | 12.39 | 8 | 2353 | CB | THR A 296 | 47.162 | 72.647 | 46.253 | 1.00 | 11.65 | 6 |
| 2312 | CB | ARG A 291 | 41.308 | 70.770 | 43.991 | 1.00 | 10.96 | 6 | 2354 | OG1 | THR A 296 | 46.005 | 73.276 | 46.812 | 1.00 | 15.42 | 8 |
| 2313 | CG | ARG A 291 | 40.602 | 69.717 | 43.110 | 1.00 | 11.39 | 6 | 2355 | CG2 | THR A 296 | 46.976 | 72.308 | 44.770 | 1.00 | 13.16 | 6 |
| 2314 | CD | ARG A 291 | 40.480 | 70.173 | 41.647 | 1.00 | 11.11 | 6 | 2356 | N | PHE A 297 | 46.760 | 71.647 | 49.472 | 1.00 | 11.24 | 7 |
| 2315 | NE | ARG A 291 | 41.729 | 70.343 | 40.907 | 1.00 | 11.15 | 7 | 2357 | CA | PHE A 297 | 46.917 | 72.026 | 50.881 | 1.00 | 12.10 | 6 |
| 2316 | CZ | ARG A 291 | 42.225 | 69.361 | 40.109 | 1.00 | 12.12 | 6 | 2358 | C | PHE A 297 | 47.104 | 73.543 | 50.984 | 1.00 | 17.18 | 6 |
| 2317 | NH1 | ARG A 291 | 41.706 | 68.126 | 40.068 | 1.00 | 11.32 | 7 | 2359 | O | PHE A 297 | 47.719 | 74.035 | 51.952 | 1.00 | 17.61 | 8 |
| 2318 | NH2 | ARG A 291 | 43.322 | 69.593 | 39.363 | 1.00 | 12.38 | 7 | 2360 | CB | PHE A 297 | 48.052 | 71.271 | 51.610 | 1.00 | 11.80 | 6 |
| 2319 | N | ASN A 292 | 41.972 | 72.204 | 46.801 | 1.00 | 12.65 | 7 | 2361 | CG | PHE A 297 | 47.630 | 69.924 | 52.199 | 1.00 | 14.38 | 6 |
| 2320 | CA | ASN A 292 | 42.894 | 73.001 | 47.653 | 1.00 | 11.32 | 6 | 2362 | CD1 | PHE A 297 | 47.153 | 68.917 | 51.385 | 1.00 | 13.09 | 6 |
| 2321 | C | ASN A 292 | 42.983 | 72.376 | 49.051 | 1.00 | 11.68 | 6 | 2363 | CD2 | PHE A 297 | 47.760 | 69.711 | 53.565 | 1.00 | 11.70 | 6 |
| 2322 | O | ASN A 292 | 44.074 | 72.565 | 49.634 | 1.00 | 11.50 | 8 | 2364 | CE1 | PHE A 297 | 46.821 | 67.656 | 51.854 | 1.00 | 12.95 | 6 |
| 2323 | CB | ASN A 292 | 42.408 | 74.471 | 47.750 | 1.00 | 11.01 | 6 | 2365 | CE2 | PHE A 297 | 47.438 | 68.444 | 54.064 | 1.00 | 12.92 | 6 |
| 2324 | CG | ASN A 292 | 42.593 | 75.238 | 46.379 | 1.00 | 14.57 | 6 | 2366 | CZ | PHE A 297 | 46.948 | 67.450 | 53.231 | 1.00 | 11.87 | 6 |
| 2325 | OD1 | ASN A 292 | 43.466 | 74.831 | 45.665 | 1.00 | 19.84 | 8 | 2367 | N | THR A 298 | 46.411 | 74.322 | 50.183 | 1.00 | 13.51 | 7 |
| 2326 | ND2 | ASN A 292 | 41.735 | 76.242 | 46.267 | 1.00 | 18.55 | 7 | 2368 | CA | THR A 298 | 46.398 | 75.773 | 50.270 | 1.00 | 13.52 | 6 |
| 2327 | N | VAL A 293 | 42.009 | 71.574 | 49.542 | 1.00 | 10.40 | 7 | 2369 | C | THR A 298 | 45.131 | 76.303 | 50.925 | 1.00 | 13.29 | 6 |
| 2328 | CA | VAL A 293 | 42.157 | 71.075 | 50.940 | 1.00 | 10.24 | 6 | 2370 | O | THR A 298 | 45.018 | 77.505 | 51.220 | 1.00 | 15.14 | 8 |
| 2329 | C | VAL A 293 | 42.861 | 69.743 | 50.969 | 1.00 | 11.21 | 6 | 2371 | CB | THR A 298 | 46.488 | 76.437 | 48.870 | 1.00 | 13.68 | 6 |
| 2330 | O | VAL A 293 | 43.748 | 69.520 | 51.783 | 1.00 | 11.98 | 8 | 2372 | OG1 | THR A 298 | 45.446 | 75.982 | 48.035 | 1.00 | 12.95 | 8 |
| 2331 | CB | VAL A 293 | 40.703 | 70.961 | 51.499 | 1.00 | 10.95 | 6 | 2373 | CG2 | THR A 298 | 47.869 | 76.059 | 48.250 | 1.00 | 15.45 | 6 |
| 2332 | CG1 | VAL A 293 | 40.707 | 70.175 | 52.820 | 1.00 | 12.97 | 6 | 2374 | N | GLN A 299 | 44.162 | 75.400 | 51.194 | 1.00 | 10.17 | 7 |
| 2333 | CG2 | VAL A 293 | 40.153 | 72.364 | 51.736 | 1.00 | 13.88 | 6 | 2375 | CA | GLN A 299 | 43.009 | 75.785 | 51.975 | 1.00 | 13.00 | 6 |
| 2334 | N | PHE A 294 | 42.479 | 68.858 | 50.033 | 1.00 | 11.12 | 7 | 2376 | C | GLN A 299 | 42.852 | 74.738 | 53.114 | 1.00 | 14.72 | 6 |
| 2335 | CA | PHE A 294 | 43.106 | 67.537 | 49.960 | 1.00 | 11.38 | 6 | 2377 | O | GLN A 299 | 43.624 | 73.753 | 53.094 | 1.00 | 14.92 | 8 |
| 2336 | C | PHE A 294 | 44.255 | 67.464 | 48.964 | 1.00 | 11.51 | 6 | 2378 | CB | GLN A 299 | 41.654 | 75.808 | 51.214 | 1.00 | 11.79 | 6 |
| 2337 | O | PHE A 294 | 45.095 | 66.540 | 49.093 | 1.00 | 11.86 | 8 | 2379 | CG | GLN A 299 | 41.692 | 77.072 | 50.299 | 1.00 | 14.80 | 6 |
| 2338 | CB | PHE A 294 | 42.063 | 66.455 | 49.553 | 1.00 | 11.70 | 6 | 2380 | CD | GLN A 299 | 40.301 | 77.320 | 49.668 | 1.00 | 16.23 | 6 |
| 2339 | CG | PHE A 294 | 40.936 | 66.334 | 50.584 | 1.00 | 11.57 | 6 | 2381 | OB1 | GLN A 299 | 39.959 | 76.525 | 48.827 | 1.00 | 15.11 | 8 |
| 2340 | CD1 | PHE A 294 | 41.178 | 65.683 | 51.808 | 1.00 | 11.48 | 6 | 2382 | NE2 | GLN A 299 | 39.635 | 78.376 | 50.107 | 1.00 | 17.75 | 7 |
| 2341 | CD2 | PHE A 294 | 39.707 | 66.865 | 50.295 | 1.00 | 13.60 | 6 | 2383 | N | THR A 300 | 42.031 | 75.020 | 54.106 | 1.00 | 13.71 | 7 |
| 2342 | CE1 | PHE A 294 | 40.133 | 65.579 | 52.724 | 1.00 | 12.41 | 6 | 2384 | CA | THR A 300 | 41.924 | 74.106 | 55.252 | 1.00 | 11.61 | 6 |
| 2343 | CE2 | PHE A 294 | 38.662 | 66.762 | 51.232 | 1.00 | 13.36 | 6 | 2385 | C | THR A 300 | 40.518 | 73.485 | 55.355 | 1.00 | 14.08 | 6 |
| 2344 | CZ | PHE A 294 | 38.880 | 66.104 | 52.463 | 1.00 | 13.22 | 6 | 2386 | O | THR A 300 | 39.580 | 73.874 | 54.644 | 1.00 | 11.91 | 8 |
| 2345 | N | GLY A 295 | 44.295 | 68.355 | 47.976 | 1.00 | 11.76 | 7 | 2387 | CB | THR A 300 | 42.152 | 74.850 | 56.601 | 1.00 | 15.34 | 6 |
| 2346 | CA | GLY A 295 | 45.328 | 68.234 | 46.907 | 1.00 | 12.36 | 6 | 2388 | OG1 | THR A 300 | 41.116 | 75.771 | 56.804 | 1.00 | 15.70 | 8 |
| 2347 | C | GLY A 295 | 46.504 | 69.187 | 47.187 | 1.00 | 10.85 | 6 | 2389 | CG2 | THR A 300 | 43.511 | 75.587 | 56.464 | 1.00 | 16.98 | 6 |
| 2348 | O | GLY A 295 | 47.547 | 68.676 | 47.612 | 1.00 | 13.29 | 8 | 2390 | N | MET A 301 | 40.337 | 72.672 | 56.443 | 1.00 | 11.88 | 7 |

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|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|----|
| 2391 | CA | MET A 301 | 38.977 | 72.123 | 56.650 | 1.00 | 12.22 | 6 | 2433 | ND2 | ASN A 305 | 31.910 | 74.651 | 58.967 | 1.00 | 17.24 | 7 |
| 2392 | C | MET A 301 | 37.972 | 73.216 | 56.994 | 1.00 | 12.44 | 6 | 2434 | N | ASN A 306 | 33.061 | 75.772 | 55.272 | 1.00 | 11.86 | 7 |
| 2393 | O | MET A 301 | 36.791 | 73.075 | 56.691 | 1.00 | 11.03 | 8 | 2435 | CA | ASN A 306 | 32.418 | 77.036 | 54.848 | 1.00 | 12.68 | 6 |
| 2394 | CB | MET A 301 | 38.935 | 71.065 | 57.800 | 1.00 | 12.80 | 6 | 2436 | C | ASN A 306 | 31.740 | 76.830 | 53.499 | 1.00 | 13.44 | 6 |
| 2395 | CG | MET A 301 | 39.707 | 69.787 | 57.393 | 1.00 | 11.05 | 6 | 2437 | O | ASN A 306 | 30.672 | 77.409 | 53.225 | 1.00 | 13.40 | 8 |
| 2396 | SD | MET A 301 | 39.027 | 69.014 | 55.895 | 1.00 | 12.28 | 16 | 2438 | CB | ASN A 306 | 33.438 | 78.176 | 54.774 | 1.00 | 12.13 | 6 |
| 2397 | CE | MET A 301 | 39.724 | 67.366 | 56.047 | 1.00 | 14.34 | 6 | 2439 | CG | ASN A 306 | 33.863 | 78.686 | 56.143 | 1.00 | 20.79 | 6 |
| 2398 | N | TYR A 302 | 38.408 | 74.374 | 57.555 | 1.00 | 12.00 | 7 | 2440 | OD1 | ASN A 306 | 33.275 | 78.499 | 57.233 | 1.00 | 23.19 | 8 |
| 2399 | CA | TYR A 302 | 37.462 | 75.453 | 57.759 | 1.00 | 10.79 | 6 | 2441 | ND2 | ASN A 306 | 34.959 | 79.477 | 56.155 | 1.00 | 24.17 | 7 |
| 2400 | C | TYR A 302 | 36.898 | 75.974 | 56.430 | 1.00 | 11.89 | 6 | 2442 | N | MET A 307 | 32.405 | 76.105 | 52.589 | 1.00 | 11.55 | 7 |
| 2401 | O | TYR A 302 | 35.694 | 76.181 | 56.325 | 1.00 | 12.65 | 8 | 2443 | CA | MET A 307 | 31.750 | 75.915 | 51.254 | 1.00 | 11.38 | 6 |
| 2402 | CB | TYR A 302 | 38.131 | 76.626 | 58.505 | 1.00 | 10.20 | 6 | 2444 | C | MET A 307 | 30.590 | 74.957 | 51.272 | 1.00 | 12.48 | 6 |
| 2403 | CG | TYR A 302 | 38.409 | 76.271 | 59.983 | 1.00 | 11.51 | 6 | 2445 | O | MET A 307 | 29.639 | 75.156 | 50.512 | 1.00 | 13.10 | 8 |
| 2404 | CD1 | TYR A 302 | 37.375 | 76.197 | 60.914 | 1.00 | 16.19 | 6 | 2446 | CB | MET A 307 | 32.849 | 75.431 | 50.252 | 1.00 | 12.11 | 6 |
| 2405 | CD2 | TYR A 302 | 39.739 | 76.057 | 60.344 | 1.00 | 17.97 | 6 | 2447 | CG | MET A 307 | 32.375 | 75.462 | 48.767 | 1.00 | 12.14 | 6 |
| 2406 | CE1 | TYR A 302 | 37.736 | 75.884 | 62.236 | 1.00 | 18.06 | 6 | 2448 | SD | MET A 307 | 31.759 | 77.075 | 48.246 | 1.00 | 12.77 | 16 |
| 2407 | CE2 | TYR A 302 | 40.062 | 75.723 | 61.683 | 1.00 | 15.93 | 6 | 2449 | CE | MET A 307 | 33.282 | 78.010 | 48.324 | 1.00 | 13.86 | 6 |
| 2408 | CZ | TYR A 302 | 39.029 | 75.670 | 62.567 | 1.00 | 19.00 | 6 | 2450 | N | VAL A 308 | 30.592 | 73.951 | 52.152 | 1.00 | 10.38 | 7 |
| 2409 | OH | TYR A 302 | 39.409 | 75.355 | 63.905 | 1.00 | 21.46 | 8 | 2451 | CA | VAL A 308 | 29.383 | 73.136 | 52.340 | 1.00 | 10.10 | 6 |
| 2410 | N | ASP A 303 | 37.763 | 76.026 | 55.418 | 1.00 | 13.06 | 7 | 2452 | C | VAL A 308 | 28.272 | 74.049 | 52.822 | 1.00 | 11.64 | 6 |
| 2411 | CA | ASP A 303 | 37.256 | 76.434 | 54.104 | 1.00 | 12.54 | 6 | 2453 | O | VAL A 308 | 27.153 | 73.974 | 52.321 | 1.00 | 13.14 | 8 |
| 2412 | C | ASP A 303 | 36.285 | 75.409 | 53.492 | 1.00 | 11.88 | 6 | 2454 | CB | VAL A 308 | 29.712 | 72.052 | 53.406 | 1.00 | 13.16 | 6 |
| 2413 | O | ASP A 303 | 35.330 | 75.782 | 52.785 | 1.00 | 13.46 | 8 | 2455 | CG1 | VAL A 308 | 28.388 | 71.356 | 53.770 | 1.00 | 14.05 | 6 |
| 2414 | CB | ASP A 303 | 38.419 | 76.666 | 53.133 | 1.00 | 10.93 | 6 | 2456 | CG2 | VAL A 308 | 30.641 | 71.038 | 52.727 | 1.00 | 13.08 | 6 |
| 2415 | CG | ASP A 303 | 39.386 | 77.734 | 53.654 | 1.00 | 14.78 | 6 | 2457 | N | ASN A 309 | 28.541 | 74.952 | 53.784 | 1.00 | 12.04 | 7 |
| 2416 | OD1 | ASP A 303 | 38.879 | 78.877 | 53.849 | 1.00 | 13.77 | 8 | 2458 | CA | ASN A 309 | 27.479 | 75.848 | 54.264 | 1.00 | 12.56 | 6 |
| 2417 | OD2 | ASP A 303 | 40.573 | 77.435 | 53.832 | 1.00 | 13.10 | 8 | 2459 | C | ASN A 309 | 27.073 | 76.824 | 53.176 | 1.00 | 13.56 | 6 |
| 2418 | N | LEU A 304 | 36.602 | 74.152 | 53.720 | 1.00 | 11.36 | 7 | 2460 | O | ASN A 309 | 25.875 | 77.017 | 53.030 | 1.00 | 15.38 | 8 |
| 2419 | CA | LEU A 304 | 35.713 | 73.086 | 53.156 | 1.00 | 11.06 | 6 | 2461 | CB | ASN A 309 | 27.997 | 76.680 | 55.470 | 1.00 | 14.00 | 6 |
| 2420 | C | LEU A 304 | 34.348 | 73.181 | 53.841 | 1.00 | 12.95 | 6 | 2462 | CG | ASN A 309 | 28.109 | 75.761 | 56.684 | 1.00 | 20.56 | 6 |
| 2421 | O | LEU A 304 | 33.315 | 73.111 | 53.155 | 1.00 | 11.60 | 8 | 2463 | OD1 | ASN A 309 | 27.432 | 74.725 | 56.748 | 1.00 | 26.71 | 8 |
| 2422 | CB | LEU A 304 | 36.393 | 71.742 | 53.367 | 1.00 | 10.48 | 6 | 2464 | ND2 | ASN A 309 | 28.967 | 76.208 | 57.595 | 1.00 | 21.18 | 7 |
| 2423 | CG | LEU A 304 | 35.687 | 70.566 | 52.633 | 1.00 | 11.09 | 6 | 2465 | N | GLN A 310 | 27.970 | 77.423 | 52.426 | 1.00 | 14.28 | 7 |
| 2424 | CD1 | LEU A 304 | 35.737 | 70.797 | 51.112 | 1.00 | 12.57 | 6 | 2466 | CA | GLN A 310 | 27.549 | 78.422 | 51.422 | 1.00 | 13.95 | 6 |
| 2425 | CD2 | LEU A 304 | 36.397 | 69.248 | 52.971 | 1.00 | 12.54 | 6 | 2467 | C | GLN A 310 | 26.734 | 77.754 | 50.319 | 1.00 | 13.50 | 6 |
| 2426 | N | ASN A 305 | 34.290 | 73.255 | 55.180 | 1.00 | 11.76 | 7 | 2468 | O | GLN A 310 | 25.672 | 78.286 | 49.942 | 1.00 | 14.03 | 8 |
| 2427 | CA | ASN A 305 | 32.999 | 73.422 | 55.887 | 1.00 | 12.74 | 6 | 2469 | CB | GLN A 310 | 28.821 | 79.123 | 50.869 | 1.00 | 14.99 | 6 |
| 2428 | C | ASN A 305 | 32.308 | 74.720 | 55.479 | 1.00 | 11.54 | 6 | 2470 | CG | GLN A 310 | 28.507 | 80.214 | 49.859 | 1.00 | 21.08 | 6 |
| 2429 | O | ASN A 305 | 31.100 | 74.673 | 55.259 | 1.00 | 13.50 | 8 | 2471 | CD | GLN A 310 | 29.734 | 81.169 | 49.819 | 1.00 | 21.08 | 6 |
| 2430 | CB | ASN A 305 | 33.331 | 73.448 | 57.405 | 1.00 | 12.22 | 6 | 2472 | OE1 | GLN A 310 | 30.875 | 80.762 | 50.019 | 1.00 | 25.61 | 8 |
| 2431 | CG | ASN A 305 | 32.014 | 73.551 | 58.210 | 1.00 | 12.84 | 6 | 2473 | NE2 | GLN A 310 | 29.417 | 82.401 | 49.600 | 1.00 | 25.23 | 7 |
| 2432 | OD1 | ASN A 305 | 31.174 | 72.669 | 58.097 | 1.00 | 13.98 | 8 | 2474 | N | THR A 311 | 27.238 | 76.630 | 49.792 | 1.00 | 11.65 | 7 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2475 | CA | THR A 311 | 26.432 | 75.983 | 48.711 | 1.00 | 11.52 | 6 | 2517 | O | LYS A 316 | 17.175 | 72.963 | 47.475 | 1.00 | 14.60 | 8 |
| 2476 | C | THR A 311 | 25.089 | 75.459 | 49.257 | 1.00 | 12.57 | 6 | 2518 | CB | LYS A 316 | 16.496 | 75.595 | 45.485 | 1.00 | 14.77 | 6 |
| 2477 | O | THR A 311 | 24.039 | 75.572 | 48.599 | 1.00 | 13.81 | 8 | 2519 | CG | LYS A 316 | 15.139 | 75.068 | 46.091 | 1.00 | 18.12 | 6 |
| 2478 | CB | THR A 311 | 27.143 | 74.754 | 48.142 | 1.00 | 12.52 | 6 | 2520 | CD | LYS A 316 | 13.982 | 75.856 | 45.565 | 1.00 | 22.24 | 6 |
| 2479 | OG1 | THR A 311 | 27.593 | 73.909 | 49.194 | 1.00 | 13.67 | 8 | 2521 | CE | LYS A 316 | 12.683 | 75.166 | 46.061 | 1.00 | 19.23 | 6 |
| 2480 | CG2 | THR A 311 | 28.426 | 75.250 | 47.375 | 1.00 | 14.32 | 6 | 2522 | NZ | LYS A 316 | 12.432 | 75.635 | 47.468 | 1.00 | 22.20 | 7 |
| 2481 | N | GLY A 312 | 25.096 | 75.107 | 50.561 | 1.00 | 11.69 | 7 | 2523 | N | TYR A 317 | 18.227 | 72.953 | 45.457 | 1.00 | 13.10 | 7 |
| 2482 | CA | GLY A 312 | 23.812 | 74.642 | 51.137 | 1.00 | 14.78 | 6 | 2524 | CA | TYR A 317 | 18.316 | 71.483 | 45.445 | 1.00 | 11.39 | 6 |
| 2483 | C | GLY A 312 | 22.800 | 75.792 | 51.223 | 1.00 | 14.32 | 6 | 2525 | C | TYR A 317 | 19.805 | 71.123 | 45.506 | 1.00 | 10.31 | 6 |
| 2484 | O | GLY A 312 | 21.573 | 75.473 | 51.276 | 1.00 | 16.33 | 8 | 2526 | O | TYR A 317 | 20.410 | 70.491 | 44.637 | 1.00 | 12.52 | 8 |
| 2485 | N | ASN A 313 | 23.320 | 76.998 | 51.476 | 1.00 | 13.08 | 7 | 2527 | CB | TYR A 317 | 17.652 | 70.893 | 44.157 | 1.00 | 12.53 | 6 |
| 2486 | CA | ASN A 313 | 22.392 | 78.108 | 51.535 | 1.00 | 13.20 | 6 | 2528 | CG | TYR A 317 | 16.221 | 71.387 | 44.004 | 1.00 | 13.61 | 6 |
| 2487 | C | ASN A 313 | 21.980 | 78.575 | 50.150 | 1.00 | 14.89 | 6 | 2529 | CD1 | TYR A 317 | 15.272 | 70.932 | 44.915 | 1.00 | 14.65 | 6 |
| 2488 | O | ASN A 313 | 20.827 | 79.097 | 50.014 | 1.00 | 20.75 | 8 | 2530 | CD2 | TYR A 317 | 15.800 | 72.280 | 43.030 | 1.00 | 14.34 | 6 |
| 2489 | CB | ASN A 313 | 23.155 | 79.260 | 52.204 | 1.00 | 19.18 | 6 | 2531 | CE1 | TYR A 317 | 13.938 | 71.366 | 44.811 | 1.00 | 13.78 | 6 |
| 2490 | CG | ASN A 313 | 23.210 | 79.024 | 53.718 | 1.00 | 30.91 | 6 | 2532 | CE2 | TYR A 317 | 14.511 | 72.767 | 42.890 | 1.00 | 12.10 | 6 |
| 2491 | OD1 | ASN A 313 | 22.384 | 78.310 | 54.281 | 1.00 | 30.04 | 8 | 2533 | CZ | TYR A 317 | 13.604 | 72.246 | 43.832 | 1.00 | 15.19 | 6 |
| 2492 | ND2 | ASN A 313 | 24.152 | 79.691 | 54.360 | 1.00 | 31.03 | 7 | 2534 | OH | TYR A 317 | 12.275 | 72.682 | 43.733 | 1.00 | 14.53 | 8 |
| 2493 | N | GLU A 314 | 22.802 | 78.394 | 49.111 | 1.00 | 12.83 | 7 | 2535 | N | LYS A 318 | 20.375 | 71.463 | 46.702 | 1.00 | 11.46 | 7 |
| 2494 | CA | GLU A 314 | 22.396 | 79.060 | 47.822 | 1.00 | 11.95 | 6 | 2536 | CA | LYS A 318 | 21.821 | 71.130 | 46.865 | 1.00 | 10.64 | 6 |
| 2495 | C | GLU A 314 | 21.621 | 78.137 | 46.889 | 1.00 | 13.20 | 6 | 2537 | O | LYS A 318 | 22.053 | 69.651 | 46.865 | 1.00 | 10.21 | 6 |
| 2496 | O | GLU A 314 | 20.733 | 78.689 | 46.175 | 1.00 | 13.02 | 8 | 2538 | C | LYS A 318 | 23.133 | 69.145 | 46.529 | 1.00 | 10.36 | 8 |
| 2497 | CB | GLU A 314 | 23.753 | 79.394 | 47.117 | 1.00 | 10.17 | 6 | 2539 | CB | LYS A 318 | 22.408 | 71.772 | 48.141 | 1.00 | 9.85 | 6 |
| 2498 | CG | GLU A 314 | 24.503 | 80.510 | 47.842 | 1.00 | 12.02 | 6 | 2540 | CG | LYS A 318 | 21.843 | 71.211 | 49.451 | 1.00 | 13.57 | 6 |
| 2499 | CD | GLU A 314 | 25.715 | 80.987 | 46.985 | 1.00 | 15.94 | 6 | 2541 | CD | LYS A 318 | 20.619 | 72.105 | 49.820 | 1.00 | 19.29 | 6 |
| 2500 | OE1 | GLU A 314 | 26.285 | 80.206 | 46.232 | 1.00 | 15.22 | 8 | 2542 | CE | LYS A 318 | 20.309 | 72.064 | 51.345 | 1.00 | 19.13 | 6 |
| 2501 | OE2 | GLU A 314 | 26.164 | 82.100 | 47.284 | 1.00 | 24.00 | 8 | 2543 | NZ | LYS A 318 | 19.066 | 72.819 | 51.636 | 1.00 | 20.57 | 7 |
| 2502 | N | TYR A 315 | 21.992 | 76.840 | 46.892 | 1.00 | 11.76 | 7 | 2544 | N | GLU A 319 | 21.044 | 68.796 | 47.174 | 1.00 | 9.32 | 7 |
| 2503 | CA | TYR A 315 | 21.297 | 75.979 | 45.885 | 1.00 | 10.85 | 6 | 2545 | CA | GLU A 319 | 21.217 | 67.359 | 47.096 | 1.00 | 11.07 | 6 |
| 2504 | C | TYR A 315 | 20.032 | 75.368 | 46.506 | 1.00 | 12.73 | 6 | 2546 | C | GLU A 319 | 21.164 | 66.802 | 45.667 | 1.00 | 12.26 | 6 |
| 2505 | O | TYR A 315 | 20.140 | 74.648 | 47.510 | 1.00 | 12.47 | 8 | 2547 | O | GLU A 319 | 21.469 | 65.627 | 45.504 | 1.00 | 11.85 | 8 |
| 2506 | CB | TYR A 315 | 22.265 | 74.838 | 45.494 | 1.00 | 12.39 | 6 | 2548 | CB | GLU A 319 | 20.021 | 66.636 | 47.827 | 1.00 | 12.74 | 6 |
| 2507 | CG | TYR A 315 | 23.437 | 75.394 | 44.699 | 1.00 | 10.41 | 6 | 2549 | CG | GLU A 319 | 19.998 | 67.027 | 49.320 | 1.00 | 15.35 | 6 |
| 2508 | CD1 | TYR A 315 | 23.270 | 75.610 | 43.316 | 1.00 | 11.23 | 6 | 2550 | CD | GLU A 319 | 19.346 | 68.353 | 49.656 | 1.00 | 19.53 | 6 |
| 2509 | CD2 | TYR A 315 | 24.613 | 75.785 | 45.297 | 1.00 | 12.52 | 6 | 2551 | OE1 | GLU A 319 | 18.645 | 68.996 | 48.818 | 1.00 | 14.20 | 8 |
| 2510 | CE1 | TYR A 315 | 24.333 | 76.166 | 44.586 | 1.00 | 12.92 | 6 | 2552 | OE2 | GLU A 319 | 19.503 | 68.829 | 50.839 | 1.00 | 14.17 | 8 |
| 2511 | CE2 | TYR A 315 | 25.686 | 76.350 | 44.563 | 1.00 | 10.90 | 6 | 2553 | N | ASN A 320 | 21.033 | 67.681 | 44.664 | 1.00 | 9.38 | 7 |
| 2512 | CZ | TYR A 315 | 25.510 | 76.507 | 43.187 | 1.00 | 12.76 | 6 | 2554 | CA | ASN A 320 | 21.155 | 67.324 | 43.285 | 1.00 | 9.77 | 6 |
| 2513 | OH | TYR A 315 | 26.595 | 77.056 | 42.517 | 1.00 | 13.74 | 8 | 2555 | C | ASN A 320 | 22.454 | 67.819 | 42.636 | 1.00 | 12.36 | 6 |
| 2514 | N | LYS A 316 | 18.895 | 75.634 | 45.861 | 1.00 | 11.54 | 7 | 2556 | O | ASN A 320 | 22.736 | 67.591 | 41.442 | 1.00 | 10.93 | 8 |
| 2515 | CA | LYS A 316 | 17.638 | 75.080 | 46.395 | 1.00 | 14.39 | 6 | 2557 | CB | ASN A 320 | 19.995 | 67.901 | 42.402 | 1.00 | 10.57 | 6 |
| 2516 | C | LYS A 316 | 17.578 | 73.555 | 46.454 | 1.00 | 15.27 | 6 | 2558 | CG | ASN A 320 | 18.660 | 67.290 | 42.784 | 1.00 | 14.03 | 6 |

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|------|---------------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 2559 | OD1 ASN A 320 | 18.619 | 66.275 | 43.445 | 1.00 | 13.17 | 8 | 2601 | CG2AILE A 325 | 37.288 | 64.325 | 44.695 | 0.60 | 12.60 | 6 |
| 2560 | ND2 ASN A 320 | 17.558 | 67.901 | 42.323 | 1.00 | 10.64 | 7 | 2602 | CD1AILE A 325 | 39.550 | 62.693 | 43.585 | 0.60 | 10.36 | 6 |
| 2561 | N LEU A 321 | 23.285 | 68.499 | 43.422 | 1.00 | 10.68 | 7 | 2599 | CB BILE A 325 | 38.139 | 64.627 | 43.330 | 0.40 | 12.90 | 6 |
| 2562 | CA LEU A 321 | 24.610 | 68.918 | 42.896 | 1.00 | 10.60 | 6 | 2600 | CG1BILE A 325 | 37.386 | 64.127 | 44.568 | 0.40 | 10.36 | 6 |
| 2563 | C LEU A 321 | 25.415 | 67.643 | 42.685 | 1.00 | 10.70 | 6 | 2601 | CG2BILE A 325 | 39.604 | 64.862 | 43.640 | 0.40 | 10.82 | 6 |
| 2564 | O LEU A 321 | 25.448 | 66.685 | 43.452 | 1.00 | 11.96 | 8 | 2602 | CD1BILE A 325 | 37.571 | 62.651 | 44.847 | 0.40 | 13.69 | 6 |
| 2565 | CB LEU A 321 | 25.299 | 69.733 | 44.024 | 1.00 | 9.53 | 6 | 2603 | N ASP A 326 | 38.028 | 65.680 | 40.350 | 1.00 | 9.63 | 7 |
| 2566 | CG LEU A 321 | 24.761 | 71.176 | 44.124 | 1.00 | 9.68 | 6 | 2604 | CA ASP A 326 | 38.762 | 65.987 | 39.107 | 1.00 | 10.15 | 6 |
| 2567 | CD1 LEU A 321 | 25.310 | 71.820 | 45.415 | 1.00 | 13.05 | 6 | 2605 | C ASP A 326 | 37.813 | 65.625 | 37.964 | 1.00 | 11.71 | 6 |
| 2568 | CD2 LEU A 321 | 25.183 | 72.064 | 42.930 | 1.00 | 9.85 | 6 | 2606 | O ASP A 326 | 36.678 | 65.102 | 38.209 | 1.00 | 10.86 | 8 |
| 2569 | N ILE A 322 | 26.185 | 67.671 | 41.566 | 1.00 | 9.04 | 7 | 2607 | CG ASP A 326 | 40.149 | 65.323 | 39.050 | 1.00 | 12.00 | 6 |
| 2570 | CA ILE A 322 | 27.014 | 66.478 | 41.265 | 1.00 | 9.68 | 6 | 2608 | CG ASP A 326 | 40.166 | 63.807 | 39.089 | 1.00 | 12.49 | 6 |
| 2571 | C ILE A 322 | 28.477 | 66.821 | 41.584 | 1.00 | 11.13 | 6 | 2609 | OD1 ASP A 326 | 39.080 | 63.207 | 38.870 | 1.00 | 12.13 | 8 |
| 2572 | O ILE A 322 | 29.071 | 67.716 | 40.935 | 1.00 | 10.40 | 8 | 2610 | OD2 ASP A 326 | 41.228 | 63.200 | 39.354 | 1.00 | 11.72 | 8 |
| 2573 | CB ILE A 322 | 26.872 | 66.118 | 39.767 | 1.00 | 10.10 | 6 | 2611 | N ASN A 327 | 38.279 | 65.749 | 36.731 | 1.00 | 9.05 | 7 |
| 2574 | CG1 ILE A 322 | 25.387 | 65.842 | 39.384 | 1.00 | 9.96 | 6 | 2612 | CA ASN A 327 | 37.486 | 65.359 | 35.569 | 1.00 | 10.52 | 6 |
| 2575 | CG2 ILE A 322 | 27.793 | 64.954 | 39.396 | 1.00 | 9.05 | 6 | 2613 | C ASN A 327 | 38.334 | 65.556 | 34.352 | 1.00 | 9.98 | 6 |
| 2576 | CD1 ILE A 322 | 24.773 | 64.698 | 40.258 | 1.00 | 9.05 | 6 | 2614 | O ASN A 327 | 39.573 | 65.686 | 34.478 | 1.00 | 11.19 | 8 |
| 2577 | N THR A 323 | 29.019 | 66.133 | 42.594 | 1.00 | 9.87 | 7 | 2615 | CB ASN A 327 | 36.177 | 66.162 | 35.432 | 1.00 | 11.56 | 6 |
| 2578 | CA THR A 323 | 30.333 | 66.524 | 43.130 | 1.00 | 8.82 | 6 | 2616 | CG ASN A 327 | 36.351 | 67.636 | 35.121 | 1.00 | 12.65 | 6 |
| 2579 | C THR A 323 | 31.433 | 65.704 | 42.453 | 1.00 | 9.73 | 6 | 2617 | OD1 ASN A 327 | 37.355 | 68.106 | 34.634 | 1.00 | 11.48 | 8 |
| 2580 | O THR A 323 | 31.218 | 64.628 | 41.902 | 1.00 | 10.64 | 8 | 2618 | ND2 ASN A 327 | 35.314 | 68.376 | 35.463 | 1.00 | 8.99 | 7 |
| 2581 | CB THR A 323 | 30.364 | 66.302 | 44.652 | 1.00 | 10.77 | 6 | 2619 | N HIS A 328 | 37.802 | 65.385 | 33.178 | 1.00 | 9.23 | 7 |
| 2582 | OG1 THR A 323 | 30.009 | 64.919 | 44.887 | 1.00 | 10.73 | 8 | 2620 | CA HIS A 328 | 38.599 | 65.393 | 31.958 | 1.00 | 11.14 | 6 |
| 2583 | CG2 THR A 323 | 29.314 | 67.237 | 45.318 | 1.00 | 10.06 | 6 | 2621 | C HIS A 328 | 39.037 | 66.779 | 31.471 | 1.00 | 11.62 | 6 |
| 2584 | N PHE A 324 | 32.660 | 66.234 | 42.559 | 1.00 | 9.44 | 7 | 2622 | O HIS A 328 | 39.744 | 66.836 | 30.450 | 1.00 | 11.55 | 8 |
| 2585 | CA PHE A 324 | 33.784 | 65.582 | 41.880 | 1.00 | 10.80 | 6 | 2623 | CB HIS A 328 | 37.726 | 64.740 | 30.844 | 1.00 | 10.61 | 6 |
| 2586 | C PHE A 324 | 35.086 | 66.205 | 42.385 | 1.00 | 9.58 | 6 | 2624 | CG HIS A 328 | 36.511 | 65.577 | 30.526 | 1.00 | 9.76 | 6 |
| 2587 | O PHE A 324 | 35.086 | 67.375 | 42.805 | 1.00 | 10.73 | 8 | 2625 | ND1 HIS A 328 | 35.652 | 65.938 | 31.572 | 1.00 | 11.58 | 7 |
| 2588 | CB PHE A 324 | 33.716 | 65.698 | 40.286 | 1.00 | 9.57 | 6 | 2626 | CD2 HIS A 328 | 36.012 | 66.093 | 29.370 | 1.00 | 11.35 | 6 |
| 2589 | CG PHE A 324 | 33.638 | 67.122 | 39.817 | 1.00 | 9.02 | 6 | 2627 | CE1 HIS A 328 | 34.648 | 66.668 | 31.066 | 1.00 | 12.44 | 6 |
| 2590 | CD1 PHE A 324 | 32.421 | 67.817 | 39.810 | 1.00 | 11.94 | 6 | 2628 | NE2 HIS A 328 | 34.853 | 66.756 | 29.733 | 1.00 | 11.88 | 7 |
| 2591 | CD2 PHE A 324 | 34.798 | 67.746 | 39.354 | 1.00 | 11.07 | 6 | 2629 | N ASP A 329 | 38.746 | 67.808 | 32.263 | 1.00 | 8.48 | 7 |
| 2592 | CE1 PHE A 324 | 32.321 | 69.142 | 39.380 | 1.00 | 11.10 | 6 | 2630 | CA ASP A 329 | 39.181 | 69.155 | 31.893 | 1.00 | 9.03 | 6 |
| 2593 | CE2 PHE A 324 | 34.683 | 69.083 | 38.926 | 1.00 | 11.33 | 6 | 2631 | C ASP A 329 | 40.073 | 69.793 | 32.960 | 1.00 | 12.15 | 6 |
| 2594 | CZ PHE A 324 | 33.498 | 69.788 | 38.931 | 1.00 | 13.68 | 6 | 2632 | O ASP A 329 | 40.388 | 71.012 | 32.883 | 1.00 | 12.94 | 8 |
| 2595 | N ILE A 325 | 36.137 | 65.385 | 42.285 | 1.00 | 9.28 | 7 | 2633 | CG ASP A 329 | 37.955 | 70.091 | 31.837 | 1.00 | 11.03 | 6 |
| 2596 | CA ILE A 325 | 37.469 | 65.879 | 42.710 | 1.00 | 9.24 | 6 | 2634 | CB ASP A 329 | 37.069 | 69.815 | 30.620 | 1.00 | 11.95 | 6 |
| 2597 | C ILE A 325 | 38.277 | 66.277 | 41.480 | 1.00 | 9.67 | 6 | 2635 | OD1 ASP A 329 | 37.477 | 69.188 | 29.617 | 1.00 | 11.39 | 8 |
| 2598 | O ILE A 325 | 39.255 | 67.116 | 41.645 | 1.00 | 10.76 | 8 | 2636 | OD2 ASP A 329 | 35.891 | 70.243 | 30.712 | 1.00 | 11.11 | 8 |
| 2599 | CB AILE A 325 | 38.211 | 64.869 | 43.596 | 0.60 | 11.75 | 6 | 2637 | N MET A 330 | 40.568 | 68.936 | 33.857 | 1.00 | 11.19 | 7 |
| 2600 | CGIAILE A 325 | 38.779 | 63.705 | 42.764 | 0.60 | 10.90 | 6 | 2638 | CA MET A 330 | 41.533 | 69.433 | 34.857 | 1.00 | 9.36 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2639 | C | MET A 330 | 42.537 | 68.330 | 35.211 | 1.00 | 9.51 | 6 | 2681 | N | SER A 335 | 48.014 | 63.857 | 40.144 | 1.00 | 11.98 | 7 |
| 2640 | O | MET A 330 | 42.224 | 67.156 | 34.927 | 1.00 | 11.47 | 8 | 2682 | CA | SER A 335 | 49.117 | 64.732 | 39.639 | 1.00 | 11.30 | 6 |
| 2641 | CB | MET A 330 | 40.858 | 70.015 | 36.111 | 1.00 | 13.17 | 6 | 2683 | C | SER A 335 | 49.115 | 66.026 | 40.421 | 1.00 | 15.22 | 8 |
| 2642 | CB | MET A 330 | 40.005 | 68.973 | 36.857 | 1.00 | 11.23 | 6 | 2684 | O | SER A 335 | 50.159 | 66.664 | 40.438 | 1.00 | 18.21 | 8 |
| 2643 | SD | MET A 330 | 39.087 | 69.743 | 38.236 | 1.00 | 12.96 | 16 | 2685 | CB | SER A 335 | 48.843 | 55.113 | 38.179 | 1.00 | 14.88 | 6 |
| 2644 | CE | MET A 330 | 37.923 | 70.706 | 37.364 | 1.00 | 13.78 | 6 | 2686 | OG | SER A 335 | 49.221 | 63.920 | 37.436 | 1.00 | 17.27 | 8 |
| 2645 | N | SER A 331 | 43.702 | 68.680 | 35.765 | 1.00 | 10.04 | 7 | 2687 | N | VAL A 336 | 48.041 | 66.315 | 41.169 | 1.00 | 11.92 | 7 |
| 2646 | CA | SER A 331 | 44.650 | 67.618 | 36.030 | 1.00 | 9.86 | 6 | 2688 | CA | VAL A 336 | 48.092 | 67.455 | 42.094 | 1.00 | 14.73 | 6 |
| 2647 | C | SER A 331 | 44.130 | 66.557 | 37.020 | 1.00 | 11.24 | 6 | 2689 | C | VAL A 336 | 48.805 | 67.064 | 43.392 | 1.00 | 15.20 | 6 |
| 2648 | O | SER A 331 | 43.295 | 66.892 | 37.858 | 1.00 | 11.71 | 8 | 2690 | O | VAL A 336 | 49.593 | 67.825 | 43.962 | 1.00 | 16.13 | 8 |
| 2649 | CB | SER A 331 | 46.009 | 68.207 | 36.629 | 1.00 | 11.21 | 6 | 2691 | CB | VAL A 336 | 46.691 | 67.970 | 42.447 | 1.00 | 14.37 | 6 |
| 2650 | OG | SER A 331 | 45.623 | 68.981 | 37.793 | 1.00 | 14.33 | 8 | 2692 | CG1 | VAL A 336 | 46.646 | 69.120 | 43.441 | 1.00 | 16.05 | 6 |
| 2651 | N | ARG A 332 | 44.540 | 65.321 | 36.833 | 1.00 | 11.49 | 7 | 2693 | CG2 | VAL A 336 | 45.970 | 68.386 | 41.154 | 1.00 | 18.05 | 6 |
| 2652 | CA | ARG A 332 | 44.057 | 64.272 | 37.749 | 1.00 | 11.49 | 6 | 2694 | N | ASN A 337 | 48.525 | 65.866 | 43.852 | 1.00 | 13.19 | 7 |
| 2653 | C | ARG A 332 | 44.499 | 64.603 | 39.189 | 1.00 | 11.63 | 6 | 2695 | CA | ASN A 337 | 49.114 | 65.389 | 45.132 | 1.00 | 12.41 | 6 |
| 2654 | O | ARG A 332 | 45.591 | 65.103 | 39.412 | 1.00 | 12.21 | 8 | 2696 | C | ASN A 337 | 49.153 | 63.870 | 44.976 | 1.00 | 12.10 | 6 |
| 2655 | CB | ARG A 332 | 44.667 | 62.914 | 37.387 | 1.00 | 13.45 | 6 | 2697 | O | ASN A 337 | 48.082 | 63.178 | 44.865 | 1.00 | 11.76 | 8 |
| 2656 | CG | ARG A 332 | 43.997 | 62.516 | 36.049 | 1.00 | 16.61 | 6 | 2698 | CB | ASN A 337 | 48.141 | 65.756 | 46.272 | 1.00 | 11.12 | 6 |
| 2657 | CD | ARG A 332 | 43.560 | 61.101 | 36.061 | 1.00 | 20.26 | 6 | 2699 | CG | ASN A 337 | 48.570 | 65.206 | 47.621 | 1.00 | 13.14 | 6 |
| 2658 | NE | ARG A 332 | 43.017 | 60.592 | 34.777 | 1.00 | 15.50 | 7 | 2700 | OD1 | ASN A 337 | 49.572 | 64.466 | 47.738 | 1.00 | 12.58 | 8 |
| 2659 | CZ | ARG A 332 | 41.965 | 59.753 | 34.882 | 1.00 | 12.48 | 6 | 2701 | ND2 | ASN A 337 | 47.865 | 65.514 | 48.694 | 1.00 | 11.19 | 7 |
| 2660 | NH1 | ARG A 332 | 41.546 | 59.388 | 36.094 | 1.00 | 10.61 | 7 | 2702 | N | SER A 338 | 50.364 | 63.275 | 44.939 | 1.00 | 9.71 | 7 |
| 2661 | NH2 | ARG A 332 | 41.440 | 59.251 | 33.741 | 1.00 | 10.74 | 7 | 2703 | CA | SER A 338 | 50.477 | 61.849 | 44.747 | 1.00 | 13.36 | 6 |
| 2662 | N | PHE A 333 | 43.654 | 64.168 | 40.153 | 1.00 | 9.55 | 7 | 2704 | C | SER A 338 | 50.257 | 60.983 | 45.993 | 1.00 | 11.43 | 6 |
| 2663 | CA | PHE A 333 | 44.019 | 64.431 | 41.533 | 1.00 | 10.54 | 6 | 2705 | O | SER A 338 | 50.294 | 59.759 | 45.858 | 1.00 | 14.29 | 8 |
| 2664 | C | PHE A 333 | 45.461 | 63.976 | 41.852 | 1.00 | 12.40 | 6 | 2706 | CB | SER A 338 | 51.884 | 61.461 | 44.225 | 1.00 | 17.19 | 6 |
| 2665 | O | PHE A 333 | 46.170 | 64.709 | 42.515 | 1.00 | 13.01 | 8 | 2707 | OG | SER A 338 | 52.871 | 61.883 | 45.154 | 1.00 | 17.12 | 8 |
| 2666 | CB | PHE A 333 | 43.007 | 63.676 | 42.481 | 1.00 | 11.67 | 6 | 2708 | N | ASN A 339 | 49.847 | 61.610 | 47.095 | 1.00 | 13.33 | 7 |
| 2667 | CG | PHE A 333 | 43.365 | 64.006 | 43.958 | 1.00 | 12.76 | 6 | 2709 | CA | ASN A 339 | 49.601 | 60.788 | 48.297 | 1.00 | 12.26 | 6 |
| 2668 | CD1 | PHE A 333 | 44.315 | 63.230 | 44.587 | 1.00 | 15.62 | 6 | 2710 | C | ASN A 339 | 48.267 | 60.043 | 48.193 | 1.00 | 12.82 | 6 |
| 2669 | CD2 | PHE A 333 | 42.718 | 65.041 | 44.556 | 1.00 | 18.86 | 6 | 2711 | O | ASN A 339 | 47.246 | 60.732 | 48.134 | 1.00 | 12.55 | 8 |
| 2670 | CE1 | PHE A 333 | 44.651 | 63.513 | 45.905 | 1.00 | 19.61 | 6 | 2712 | CB | ASN A 339 | 49.554 | 61.769 | 49.485 | 1.00 | 10.37 | 6 |
| 2671 | CE2 | PHE A 333 | 43.014 | 65.342 | 45.906 | 1.00 | 15.77 | 6 | 2713 | CG | ASN A 339 | 49.516 | 60.949 | 50.787 | 1.00 | 18.65 | 6 |
| 2672 | CZ | PHE A 333 | 43.978 | 64.561 | 46.492 | 1.00 | 16.46 | 6 | 2714 | OD1 | ASN A 339 | 48.403 | 60.509 | 51.110 | 1.00 | 19.28 | 8 |
| 2673 | CA | LEU A 334 | 45.825 | 62.763 | 41.462 | 1.00 | 10.49 | 7 | 2715 | ND2 | ASN A 339 | 50.648 | 60.809 | 51.502 | 1.00 | 18.28 | 7 |
| 2674 | N | LEU A 334 | 47.183 | 62.257 | 41.835 | 1.00 | 14.60 | 6 | 2716 | N | LYS A 340 | 48.283 | 58.708 | 48.148 | 1.00 | 12.73 | 7 |
| 2675 | C | LEU A 334 | 48.303 | 63.035 | 41.167 | 1.00 | 12.74 | 6 | 2717 | CA | LYS A 340 | 47.008 | 58.021 | 47.941 | 1.00 | 11.20 | 6 |
| 2676 | O | LEU A 334 | 49.456 | 62.864 | 41.627 | 1.00 | 13.05 | 8 | 2718 | C | LYS A 340 | 46.077 | 58.134 | 49.122 | 1.00 | 13.56 | 6 |
| 2677 | CB | LEU A 334 | 47.269 | 60.748 | 41.476 | 1.00 | 13.94 | 6 | 2719 | O | LYS A 340 | 44.859 | 58.103 | 48.906 | 1.00 | 12.59 | 8 |
| 2678 | CG | LEU A 334 | 46.461 | 59.910 | 42.484 | 1.00 | 13.29 | 6 | 2720 | CB | LYS A 340 | 47.345 | 56.523 | 47.665 | 1.00 | 12.59 | 6 |
| 2679 | CD1 | LEU A 334 | 46.488 | 58.447 | 41.969 | 1.00 | 14.98 | 6 | 2721 | CG | LYS A 340 | 48.006 | 56.401 | 46.279 | 1.00 | 12.90 | 6 |
| 2680 | CD2 | LEU A 334 | 47.045 | 59.905 | 43.909 | 1.00 | 13.51 | 6 | 2722 | CD | LYS A 340 | 48.318 | 54.903 | 46.055 | 1.00 | 18.47 | 6 |

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|------|-----|-----------|--------|--------|--------|------------|---|------|-----|-----------|--------|--------|--------|------------|---|
| 2723 | CE | LVS A 340 | 48.937 | 54.658 | 44.699 | 1.00 18.65 | 6 | 2765 | N | ALA A 346 | 39.590 | 62.418 | 49.883 | 1.00 11.81 | 7 |
| 2724 | NZ | LVS A 340 | 50.377 | 55.099 | 44.564 | 1.00 22.63 | 7 | 2766 | CA | ALA A 346 | 38.762 | 63.250 | 48.987 | 1.00 10.44 | 5 |
| 2725 | N | ALA A 341 | 46.585 | 58.363 | 50.345 | 1.00 12.85 | 7 | 2767 | C | ALA A 346 | 37.604 | 62.379 | 48.462 | 1.00 11.17 | 6 |
| 2726 | CA | ALA A 341 | 45.626 | 58.557 | 51.453 | 1.00 14.45 | 6 | 2768 | O | ALA A 346 | 36.473 | 62.887 | 48.339 | 1.00 11.30 | 8 |
| 2727 | C | ALA A 341 | 44.835 | 59.830 | 51.239 | 1.00 13.48 | 6 | 2769 | CB | ALA A 346 | 39.595 | 63.827 | 47.829 | 1.00 9.34 | 6 |
| 2728 | O | ALA A 341 | 43.661 | 59.855 | 51.568 | 1.00 11.31 | 8 | 2770 | N | LEU A 347 | 37.895 | 61.107 | 48.079 | 1.00 12.34 | 7 |
| 2729 | CB | ALA A 341 | 46.346 | 58.628 | 52.806 | 1.00 15.23 | 6 | 2771 | CA | LEU A 347 | 36.809 | 60.261 | 47.589 | 1.00 11.12 | 5 |
| 2730 | N | ASN A 342 | 45.459 | 60.911 | 50.731 | 1.00 10.37 | 7 | 2772 | C | LEU A 347 | 35.777 | 59.999 | 48.733 | 1.00 9.98 | 6 |
| 2731 | CA | ASN A 342 | 44.717 | 62.126 | 50.470 | 1.00 10.38 | 6 | 2773 | O | LEU A 347 | 34.567 | 60.087 | 48.466 | 1.00 11.63 | 8 |
| 2732 | C | ASN A 342 | 43.687 | 61.897 | 49.359 | 1.00 10.62 | 6 | 2774 | CB | LEU A 347 | 37.367 | 58.885 | 47.187 | 1.00 11.26 | 6 |
| 2733 | O | ASN A 342 | 42.560 | 62.477 | 49.439 | 1.00 12.01 | 8 | 2775 | CG | LEU A 347 | 38.146 | 58.913 | 45.840 | 1.00 14.75 | 6 |
| 2734 | CB | ASN A 342 | 45.708 | 63.276 | 50.141 | 1.00 11.46 | 6 | 2776 | CD1 | LEU A 347 | 38.829 | 57.574 | 45.530 | 1.00 13.09 | 6 |
| 2735 | CG | ASN A 342 | 46.519 | 63.737 | 51.351 | 1.00 13.17 | 6 | 2777 | CD2 | LEU A 347 | 37.132 | 59.197 | 44.722 | 1.00 15.41 | 6 |
| 2736 | OD1 | ASN A 342 | 47.710 | 64.044 | 51.127 | 1.00 12.82 | 8 | 2778 | N | ALA A 348 | 36.304 | 59.764 | 49.955 | 1.00 10.14 | 7 |
| 2737 | ND2 | ASN A 342 | 45.888 | 63.859 | 52.516 | 1.00 12.05 | 7 | 2779 | CA | ALA A 348 | 35.269 | 59.479 | 51.003 | 1.00 10.67 | 6 |
| 2738 | N | LEU A 343 | 44.001 | 61.049 | 48.344 | 1.00 10.66 | 7 | 2780 | C | ALA A 348 | 34.432 | 60.725 | 51.273 | 1.00 12.22 | 6 |
| 2739 | CA | LEU A 343 | 42.953 | 60.715 | 47.377 | 1.00 10.18 | 6 | 2781 | O | ALA A 348 | 33.231 | 60.600 | 51.534 | 1.00 11.88 | 8 |
| 2740 | C | LEU A 343 | 41.810 | 59.935 | 48.039 | 1.00 12.28 | 6 | 2782 | CB | ALA A 348 | 36.008 | 59.130 | 52.310 | 1.00 10.16 | 6 |
| 2741 | O | LEU A 343 | 40.635 | 60.288 | 47.781 | 1.00 11.44 | 8 | 2783 | N | PHE A 349 | 35.026 | 61.922 | 51.160 | 1.00 10.08 | 7 |
| 2742 | CB | LEU A 343 | 43.581 | 59.854 | 46.229 | 1.00 10.02 | 6 | 2784 | CA | PHE A 349 | 34.258 | 63.149 | 51.330 | 1.00 10.26 | 6 |
| 2743 | CG | LEU A 343 | 42.546 | 59.182 | 45.295 | 1.00 10.27 | 6 | 2785 | C | PHE A 349 | 33.120 | 63.213 | 50.282 | 1.00 9.67 | 6 |
| 2744 | CD1 | LEU A 343 | 41.847 | 60.288 | 44.550 | 1.00 13.59 | 6 | 2786 | O | PHE A 349 | 31.942 | 63.422 | 50.717 | 1.00 11.25 | 8 |
| 2745 | CD2 | LEU A 343 | 43.309 | 58.294 | 44.283 | 1.00 12.64 | 6 | 2787 | CB | PHE A 349 | 35.270 | 64.348 | 51.200 | 1.00 9.92 | 6 |
| 2746 | N | HIS A 344 | 42.173 | 58.977 | 48.898 | 1.00 11.47 | 7 | 2788 | CG | PHE A 349 | 34.515 | 65.659 | 51.357 | 1.00 8.60 | 6 |
| 2747 | CA | HIS A 344 | 41.093 | 58.185 | 49.570 | 1.00 11.49 | 6 | 2789 | CD1 | PHE A 349 | 34.016 | 66.030 | 52.605 | 1.00 11.80 | 6 |
| 2748 | C | HIS A 344 | 40.189 | 59.122 | 50.370 | 1.00 13.40 | 6 | 2790 | CD2 | PHE A 349 | 34.340 | 66.526 | 50.249 | 1.00 11.51 | 6 |
| 2749 | O | HIS A 344 | 38.951 | 58.916 | 50.500 | 1.00 12.11 | 8 | 2791 | CE1 | PHE A 349 | 33.296 | 67.247 | 52.714 | 1.00 11.90 | 6 |
| 2750 | CB | HIS A 344 | 41.731 | 57.075 | 50.439 | 1.00 9.09 | 6 | 2792 | CE2 | PHE A 349 | 33.638 | 67.709 | 50.409 | 1.00 10.49 | 6 |
| 2751 | CG | HIS A 344 | 42.520 | 56.064 | 49.656 | 1.00 10.04 | 6 | 2793 | CZ | PHE A 349 | 33.069 | 68.068 | 51.660 | 1.00 12.88 | 6 |
| 2752 | ND1 | HIS A 344 | 43.612 | 55.436 | 50.199 | 1.00 12.75 | 7 | 2794 | N | ILE A 350 | 33.411 | 63.030 | 49.005 | 1.00 8.49 | 7 |
| 2753 | CD2 | HIS A 344 | 42.363 | 55.580 | 48.370 | 1.00 11.63 | 6 | 2795 | CA | ILE A 350 | 32.257 | 63.124 | 48.089 | 1.00 10.97 | 6 |
| 2754 | CE1 | HIS A 344 | 44.114 | 54.612 | 49.289 | 1.00 10.72 | 6 | 2796 | C | ILE A 350 | 31.361 | 61.899 | 48.158 | 1.00 11.48 | 6 |
| 2755 | NE2 | HIS A 344 | 43.393 | 54.662 | 48.157 | 1.00 12.61 | 7 | 2797 | O | ILE A 350 | 30.139 | 62.115 | 47.958 | 1.00 11.30 | 8 |
| 2756 | N | GLN A 345 | 40.834 | 60.100 | 51.024 | 1.00 10.53 | 7 | 2798 | CB | ILE A 350 | 32.676 | 63.380 | 46.605 | 1.00 11.26 | 6 |
| 2757 | CA | GLN A 345 | 40.049 | 61.036 | 51.831 | 1.00 10.43 | 6 | 2799 | CG1 | ILE A 350 | 33.451 | 62.279 | 45.983 | 1.00 11.16 | 6 |
| 2758 | C | GLN A 345 | 39.077 | 61.999 | 51.008 | 1.00 10.42 | 6 | 2800 | CG2 | ILE A 350 | 33.429 | 64.742 | 46.556 | 1.00 12.07 | 6 |
| 2759 | O | GLN A 345 | 37.888 | 62.067 | 51.324 | 1.00 10.38 | 8 | 2801 | CD1 | ILE A 350 | 33.748 | 62.454 | 44.463 | 1.00 9.59 | 6 |
| 2760 | CB | GLN A 345 | 40.996 | 62.012 | 52.564 | 1.00 11.01 | 6 | 2802 | N | LEU A 351 | 31.873 | 60.731 | 48.548 | 1.00 9.78 | 7 |
| 2761 | CG | GLN A 345 | 41.847 | 61.258 | 53.641 | 1.00 9.73 | 6 | 2803 | CA | LEU A 351 | 30.930 | 59.601 | 48.655 | 1.00 9.90 | 6 |
| 2762 | CD | GLN A 345 | 43.142 | 62.041 | 53.786 | 1.00 10.78 | 6 | 2804 | C | LEU A 351 | 29.956 | 59.782 | 49.809 | 1.00 11.10 | 6 |
| 2763 | OE1 | GLN A 345 | 43.232 | 63.196 | 53.279 | 1.00 12.69 | 8 | 2805 | O | LEU A 351 | 28.888 | 59.122 | 49.698 | 1.00 11.60 | 8 |
| 2764 | NE2 | GLN A 345 | 44.170 | 61.448 | 54.428 | 1.00 12.87 | 7 | 2806 | CB | LEU A 351 | 31.813 | 58.349 | 48.879 | 1.00 11.35 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 2807 | CG | LEU A 351 | 32.492 | 57.907 | 47.564 | 1.00 | 10.64 | 6 | 2849 | CB | PRO A 357 | 30.340 | 61.021 | 44.494 | 1.00 | 10.57 | 6 |
| 2808 | CD1 | LEU A 351 | 33.679 | 56.944 | 47.822 | 1.00 | 12.51 | 6 | 2850 | CG | PRO A 357 | 29.245 | 59.991 | 44.834 | 1.00 | 11.58 | 6 |
| 2809 | CD2 | LEU A 351 | 31.500 | 57.262 | 46.595 | 1.00 | 13.68 | 6 | 2851 | CD | PRO A 357 | 27.914 | 60.760 | 44.914 | 1.00 | 10.88 | 6 |
| 2810 | N | THR A 352 | 30.267 | 60.590 | 50.850 | 1.00 | 9.74 | 7 | 2852 | N | SER A 358 | 30.508 | 62.051 | 41.293 | 1.00 | 8.23 | 7 |
| 2811 | CA | THR A 352 | 29.310 | 60.657 | 51.960 | 1.00 | 11.34 | 6 | 2853 | CA | SER A 358 | 31.003 | 61.558 | 40.001 | 1.00 | 9.73 | 6 |
| 2812 | C | THR A 352 | 28.658 | 62.022 | 52.149 | 1.00 | 12.86 | 6 | 2854 | C | SER A 358 | 32.509 | 61.272 | 40.069 | 1.00 | 10.56 | 6 |
| 2813 | O | THR A 352 | 27.822 | 62.214 | 53.022 | 1.00 | 13.09 | 8 | 2855 | O | SER A 358 | 33.323 | 62.183 | 40.331 | 1.00 | 11.97 | 8 |
| 2814 | CB | THR A 352 | 30.099 | 60.375 | 53.296 | 1.00 | 11.44 | 6 | 2856 | CB | SER A 358 | 30.768 | 62.634 | 38.921 | 1.00 | 12.36 | 6 |
| 2815 | OG1 | THR A 352 | 31.244 | 61.234 | 53.420 | 1.00 | 11.08 | 8 | 2857 | OG | SER A 358 | 31.301 | 62.159 | 37.653 | 1.00 | 13.42 | 8 |
| 2816 | CG2 | THR A 352 | 30.607 | 58.939 | 53.324 | 1.00 | 9.52 | 6 | 2858 | N | ILE A 359 | 32.813 | 59.992 | 39.915 | 1.00 | 9.37 | 7 |
| 2817 | N | SER A 353 | 29.100 | 63.028 | 51.368 | 1.00 | 10.03 | 7 | 2859 | CA | ILE A 359 | 34.234 | 59.557 | 39.927 | 1.00 | 9.47 | 6 |
| 2818 | CA | SER A 353 | 28.530 | 64.357 | 51.432 | 1.00 | 10.73 | 6 | 2860 | C | ILE A 359 | 34.703 | 59.350 | 38.492 | 1.00 | 12.04 | 6 |
| 2819 | C | SER A 353 | 27.299 | 64.574 | 50.536 | 1.00 | 9.28 | 6 | 2861 | O | ILE A 359 | 34.101 | 58.730 | 37.647 | 1.00 | 11.59 | 8 |
| 2820 | O | SER A 353 | 26.990 | 63.688 | 49.726 | 1.00 | 13.31 | 8 | 2862 | CB | ILE A 359 | 34.313 | 58.205 | 40.671 | 1.00 | 11.89 | 6 |
| 2821 | CB | SER A 353 | 29.607 | 65.403 | 51.012 | 1.00 | 12.91 | 6 | 2863 | CG1 | ILE A 359 | 33.858 | 58.478 | 42.145 | 1.00 | 14.90 | 6 |
| 2822 | OG | SER A 353 | 30.626 | 65.402 | 52.045 | 1.00 | 12.40 | 8 | 2864 | CG2 | ILE A 359 | 35.727 | 57.624 | 40.550 | 1.00 | 12.39 | 6 |
| 2823 | N | ARG A 354 | 26.646 | 65.741 | 50.754 | 1.00 | 10.25 | 7 | 2865 | CD1 | ILE A 359 | 33.936 | 57.155 | 42.925 | 1.00 | 22.17 | 6 |
| 2824 | CA | ARG A 354 | 25.379 | 65.920 | 50.024 | 1.00 | 10.03 | 6 | 2866 | N | TYR A 360 | 35.810 | 60.088 | 38.176 | 1.00 | 9.52 | 7 |
| 2825 | C | ARG A 354 | 25.611 | 65.997 | 48.533 | 1.00 | 10.84 | 6 | 2867 | CA | TYR A 360 | 36.364 | 60.076 | 36.807 | 1.00 | 8.41 | 6 |
| 2826 | O | ARG A 354 | 26.704 | 66.369 | 48.085 | 1.00 | 11.59 | 8 | 2868 | C | TYR A 360 | 37.027 | 58.709 | 36.636 | 1.00 | 9.86 | 6 |
| 2827 | CB | ARG A 354 | 24.669 | 67.185 | 50.545 | 1.00 | 10.71 | 6 | 2869 | O | TYR A 360 | 37.780 | 58.227 | 37.510 | 1.00 | 10.81 | 8 |
| 2828 | CG | ARG A 354 | 25.099 | 68.504 | 49.838 | 1.00 | 11.61 | 6 | 2870 | CB | TYR A 360 | 37.399 | 61.247 | 36.796 | 1.00 | 9.51 | 6 |
| 2829 | CD | ARG A 354 | 26.535 | 68.853 | 50.229 | 1.00 | 12.49 | 7 | 2871 | CG | TYR A 360 | 37.935 | 61.510 | 35.363 | 1.00 | 9.64 | 6 |
| 2830 | NE | ARG A 354 | 26.964 | 70.130 | 49.548 | 1.00 | 12.69 | 7 | 2872 | CD1 | TYR A 360 | 37.191 | 61.428 | 34.206 | 1.00 | 10.11 | 6 |
| 2831 | CZ | ARG A 354 | 27.455 | 70.157 | 48.317 | 1.00 | 12.54 | 6 | 2873 | CD2 | TYR A 360 | 39.279 | 61.882 | 35.294 | 1.00 | 9.54 | 6 |
| 2832 | NH1 | ARG A 354 | 27.638 | 69.113 | 47.497 | 1.00 | 12.15 | 7 | 2874 | CE1 | TYR A 360 | 37.818 | 61.650 | 32.960 | 1.00 | 10.79 | 6 |
| 2833 | NH2 | ARG A 354 | 27.867 | 71.370 | 47.894 | 1.00 | 11.14 | 7 | 2875 | CE2 | TYR A 360 | 39.927 | 62.148 | 34.066 | 1.00 | 10.73 | 6 |
| 2834 | N | GLY A 355 | 24.542 | 65.707 | 47.780 | 1.00 | 11.00 | 7 | 2876 | CZ | TYR A 360 | 39.153 | 62.044 | 32.937 | 1.00 | 11.36 | 6 |
| 2835 | CA | GLY A 355 | 24.624 | 65.584 | 46.318 | 1.00 | 10.49 | 6 | 2877 | OH | TYR A 360 | 39.712 | 62.217 | 31.670 | 1.00 | 10.12 | 8 |
| 2836 | C | GLY A 355 | 25.149 | 64.196 | 45.929 | 1.00 | 13.18 | 6 | 2878 | N | TYR A 361 | 36.808 | 58.146 | 35.418 | 1.00 | 10.09 | 7 |
| 2837 | O | GLY A 355 | 25.154 | 63.299 | 46.788 | 1.00 | 15.74 | 8 | 2879 | CA | TYR A 361 | 37.279 | 56.773 | 35.210 | 1.00 | 10.66 | 6 |
| 2838 | N | THR A 356 | 25.546 | 64.007 | 44.688 | 1.00 | 10.24 | 7 | 2880 | C | TYR A 361 | 38.748 | 56.616 | 35.593 | 1.00 | 11.54 | 6 |
| 2839 | CA | THR A 356 | 25.885 | 62.648 | 44.202 | 1.00 | 10.01 | 6 | 2881 | O | TYR A 361 | 39.556 | 57.488 | 35.297 | 1.00 | 11.37 | 8 |
| 2840 | C | THR A 356 | 27.279 | 62.722 | 43.581 | 1.00 | 10.67 | 6 | 2882 | CB | TYR A 361 | 37.051 | 56.287 | 33.730 | 1.00 | 9.71 | 6 |
| 2841 | O | THR A 356 | 27.512 | 63.621 | 42.769 | 1.00 | 10.61 | 8 | 2883 | CG | TYR A 361 | 38.086 | 56.846 | 32.765 | 1.00 | 10.50 | 6 |
| 2842 | CB | THR A 356 | 24.908 | 62.301 | 43.066 | 1.00 | 13.21 | 6 | 2884 | CD1 | TYR A 361 | 37.937 | 58.150 | 32.332 | 1.00 | 10.91 | 6 |
| 2843 | OG1 | THR A 356 | 23.622 | 62.052 | 43.698 | 1.00 | 11.93 | 8 | 2885 | CD2 | TYR A 361 | 39.176 | 56.052 | 32.383 | 1.00 | 10.62 | 6 |
| 2844 | CG2 | THR A 356 | 25.332 | 60.948 | 42.433 | 1.00 | 11.53 | 6 | 2886 | CE1 | TYR A 361 | 38.913 | 58.715 | 31.480 | 1.00 | 10.92 | 6 |
| 2845 | N | PRO A 357 | 28.184 | 61.868 | 43.967 | 1.00 | 10.42 | 7 | 2887 | CE2 | TYR A 361 | 40.155 | 56.601 | 31.520 | 1.00 | 9.87 | 6 |
| 2846 | CA | PRO A 357 | 29.564 | 61.929 | 43.493 | 1.00 | 10.52 | 6 | 2888 | CZ | TYR A 361 | 39.988 | 57.930 | 31.139 | 1.00 | 12.35 | 6 |
| 2847 | C | PRO A 357 | 29.689 | 61.366 | 42.092 | 1.00 | 11.14 | 6 | 2889 | OH | TYR A 361 | 40.982 | 58.482 | 30.297 | 1.00 | 11.60 | 8 |
| 2848 | O | PRO A 357 | 29.074 | 60.379 | 41.752 | 1.00 | 11.48 | 8 | 2890 | N | GLY A 362 | 39.069 | 55.475 | 36.171 | 1.00 | 11.61 | 7 |

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|------|-----|-----------|--------|--------|--------|------------|---|------|-----|------------|--------|--------|--------|------------|----|
| 2891 | CA | GLY A 362 | 40.454 | 55.099 | 36.513 | 1.00 12.01 | 6 | 2933 | C | MET A 367 | 46.195 | 58.365 | 37.586 | 1.00 14.58 | 6 |
| 2892 | C | GLY A 362 | 40.997 | 55.744 | 37.772 | 1.00 11.04 | 6 | 2934 | O | MET A 367 | 45.501 | 59.019 | 38.383 | 1.00 14.18 | 8 |
| 2893 | O | GLY A 362 | 42.168 | 55.431 | 38.093 | 1.00 12.36 | 8 | 2935 | CB | MET A 367 | 44.602 | 57.163 | 36.115 | 1.00 11.31 | 6 |
| 2894 | N | THR A 363 | 40.222 | 56.614 | 38.446 | 1.00 12.35 | 7 | 2936 | CG | MET A 367 | 44.316 | 55.810 | 35.397 | 1.00 11.19 | 6 |
| 2895 | CA | THR A 363 | 40.676 | 57.169 | 39.736 | 1.00 11.24 | 6 | 2937 | SD | MET A 367 | 42.994 | 56.012 | 34.139 | 1.00 13.40 | 16 |
| 2896 | C | THR A 363 | 41.033 | 56.009 | 40.693 | 1.00 11.33 | 6 | 2938 | CE | MET A 367 | 43.986 | 56.859 | 32.873 | 1.00 13.82 | 6 |
| 2897 | O | THR A 363 | 42.072 | 56.074 | 41.376 | 1.00 12.29 | 8 | 2939 | N | ALA A 368 | 47.271 | 58.817 | 36.904 | 1.00 12.72 | 7 |
| 2898 | CB | THR A 363 | 39.528 | 57.957 | 40.387 | 1.00 11.07 | 6 | 2940 | CA | ALA A 368 | 47.689 | 60.193 | 37.152 | 1.00 14.30 | 6 |
| 2899 | OG1 | THR A 363 | 39.248 | 59.065 | 39.494 | 1.00 12.04 | 8 | 2941 | C | ALA A 368 | 47.745 | 60.849 | 35.754 | 1.00 14.06 | 6 |
| 2900 | CG2 | THR A 363 | 40.024 | 58.554 | 41.730 | 1.00 11.22 | 6 | 2942 | O | ALA A 368 | 47.702 | 60.187 | 34.694 | 1.00 19.49 | 8 |
| 2901 | N | GLU A 364 | 40.221 | 54.961 | 40.670 | 1.00 11.97 | 7 | 2943 | CB | ALA A 368 | 49.047 | 60.184 | 37.904 | 1.00 15.40 | 6 |
| 2902 | CA | GLU A 364 | 40.379 | 53.835 | 41.610 | 1.00 11.29 | 6 | 2944 | N | GLY A 369 | 47.908 | 62.152 | 35.729 | 1.00 14.57 | 7 |
| 2903 | C | GLU A 364 | 41.520 | 52.938 | 41.198 | 1.00 12.77 | 6 | 2945 | CA | GLY A 369 | 48.101 | 62.780 | 34.408 | 1.00 15.04 | 6 |
| 2904 | O | GLU A 364 | 41.845 | 51.968 | 41.915 | 1.00 14.39 | 8 | 2946 | C | GLY A 369 | 47.715 | 64.242 | 34.571 | 1.00 16.47 | 6 |
| 2905 | CB | GLU A 364 | 38.994 | 53.093 | 41.712 | 1.00 10.27 | 6 | 2947 | O | GLY A 369 | 46.895 | 64.643 | 35.433 | 1.00 13.93 | 8 |
| 2906 | CG | GLU A 364 | 38.652 | 52.265 | 40.469 | 1.00 11.76 | 6 | 2948 | N | GLY A 370 | 48.524 | 65.045 | 33.872 | 1.00 12.36 | 7 |
| 2907 | CD | GLU A 364 | 38.139 | 53.001 | 39.248 | 1.00 15.28 | 6 | 2949 | CA | GLY A 370 | 48.282 | 66.487 | 33.864 | 1.00 15.60 | 6 |
| 2908 | OE1 | GLU A 364 | 38.072 | 54.257 | 39.239 | 1.00 13.43 | 8 | 2950 | C | GLY A 370 | 47.034 | 66.898 | 33.102 | 1.00 14.31 | 6 |
| 2909 | OE2 | GLU A 364 | 37.813 | 52.343 | 38.247 | 1.00 11.75 | 8 | 2951 | O | GLY A 370 | 46.202 | 66.015 | 32.888 | 1.00 18.42 | 8 |
| 2910 | N | GLN A 365 | 42.046 | 53.105 | 39.993 | 1.00 10.80 | 7 | 2952 | N | ASN A 371 | 46.994 | 68.167 | 32.710 | 1.00 14.57 | 7 |
| 2911 | CA | GLN A 365 | 43.256 | 52.398 | 39.542 | 1.00 11.28 | 6 | 2953 | CA | ASN A 371 | 45.708 | 68.579 | 32.081 | 1.00 14.92 | 6 |
| 2912 | C | GLN A 365 | 44.462 | 53.305 | 39.629 | 1.00 12.82 | 6 | 2954 | C | ASN A 371 | 45.594 | 68.064 | 30.645 | 1.00 14.23 | 6 |
| 2913 | O | GLN A 365 | 45.606 | 52.953 | 39.219 | 1.00 12.70 | 8 | 2955 | O | ASN A 371 | 46.556 | 67.570 | 30.084 | 1.00 14.23 | 8 |
| 2914 | CB | GLN A 365 | 43.138 | 51.923 | 38.088 | 1.00 12.65 | 6 | 2956 | CB | ASN A 371 | 45.420 | 70.051 | 32.240 | 0.60 23.78 | 6 |
| 2915 | CG | GLN A 365 | 41.964 | 50.951 | 37.828 | 1.00 9.91 | 6 | 2957 | CG | ASN A 371 | 43.956 | 70.451 | 32.279 | 0.60 25.40 | 6 |
| 2916 | CD | GLN A 365 | 42.043 | 49.690 | 38.593 | 1.00 14.70 | 6 | 2958 | OD1 | ASN A 371 | 43.002 | 69.778 | 31.899 | 0.60 11.28 | 8 |
| 2917 | OE1 | GLN A 365 | 41.016 | 49.200 | 39.269 | 1.00 17.54 | 8 | 2959 | ND2 | ASN A 371 | 43.728 | 71.695 | 32.756 | 0.60 26.08 | 7 |
| 2918 | NE2 | GLN A 365 | 43.204 | 49.142 | 38.847 | 1.00 12.05 | 7 | 2956 | CB | ASN A 371 | 45.872 | 70.115 | 31.871 | 0.40 16.79 | 6 |
| 2919 | N | TYR A 366 | 44.317 | 54.426 | 40.333 | 1.00 10.84 | 7 | 2957 | CG | BASN A 371 | 44.590 | 70.670 | 32.513 | 0.40 29.87 | 6 |
| 2920 | CA | TYR A 366 | 45.443 | 55.357 | 40.582 | 1.00 10.38 | 6 | 2958 | OD1 | BASN A 371 | 43.560 | 70.829 | 31.849 | 0.40 28.56 | 8 |
| 2921 | C | TYR A 366 | 46.039 | 55.921 | 39.308 | 1.00 13.18 | 6 | 2959 | ND2 | BASN A 371 | 44.801 | 70.909 | 33.793 | 0.40 23.38 | 7 |
| 2922 | O | TYR A 366 | 47.248 | 56.182 | 39.205 | 1.00 14.90 | 8 | 2960 | N | ASP A 372 | 44.373 | 68.230 | 30.152 | 1.00 12.86 | 7 |
| 2923 | CB | TYR A 366 | 46.547 | 54.753 | 41.514 | 1.00 11.57 | 6 | 2961 | CA | ASP A 372 | 44.018 | 67.780 | 28.792 | 1.00 12.97 | 6 |
| 2924 | CB | TYR A 366 | 45.872 | 54.326 | 42.813 | 1.00 11.25 | 6 | 2962 | C | ASP A 372 | 45.054 | 67.942 | 27.745 | 1.00 12.07 | 6 |
| 2925 | CD1 | TYR A 366 | 45.270 | 55.215 | 43.707 | 1.00 14.66 | 6 | 2963 | O | ASP A 372 | 45.503 | 69.093 | 27.614 | 1.00 13.32 | 8 |
| 2926 | CD2 | TYR A 366 | 45.942 | 52.977 | 43.139 | 1.00 13.34 | 6 | 2964 | CB | ASP A 372 | 42.737 | 68.624 | 28.451 | 1.00 10.31 | 6 |
| 2927 | CE1 | TYR A 366 | 44.653 | 54.747 | 44.882 | 1.00 15.95 | 6 | 2965 | CG | ASP A 372 | 42.153 | 68.351 | 27.084 | 1.00 11.02 | 6 |
| 2928 | CE2 | TYR A 366 | 45.361 | 52.494 | 44.332 | 1.00 14.89 | 6 | 2966 | OD1 | ASP A 372 | 42.556 | 67.384 | 26.464 | 1.00 12.81 | 8 |
| 2929 | CZ | TYR A 366 | 44.711 | 53.395 | 45.154 | 1.00 12.93 | 6 | 2967 | OD2 | ASP A 372 | 41.293 | 69.190 | 26.659 | 1.00 12.58 | 8 |
| 2930 | OH | TYR A 366 | 44.118 | 52.939 | 46.302 | 1.00 12.26 | 8 | 2968 | N | PRO A 373 | 45.561 | 66.874 | 27.151 | 1.00 11.77 | 7 |
| 2931 | N | MET A 367 | 45.147 | 56.315 | 38.357 | 1.00 12.15 | 7 | 2969 | CA | PRO A 373 | 44.932 | 65.582 | 26.928 | 1.00 11.70 | 6 |
| 2932 | CA | MET A 367 | 45.700 | 56.998 | 37.181 | 1.00 10.89 | 6 | 2970 | C | PRO A 373 | 45.436 | 64.544 | 27.918 | 1.00 11.76 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|----|
| 2971 | O | PRO A 373 | 45.014 | 63.392 | 27.879 | 1.00 | 11.30 | 8 | 3013 | O | MET A 378 | 44.769 | 53.836 | 30.804 | 1.00 | 12.80 | 8 |
| 2972 | CB | PRO A 373 | 45.237 | 65.136 | 25.475 | 1.00 | 10.91 | 6 | 3014 | CB | MET A 378 | 44.714 | 53.606 | 27.749 | 1.00 | 13.64 | 6 |
| 2973 | CG | PRO A 373 | 46.632 | 65.755 | 25.353 | 1.00 | 14.12 | 6 | 3015 | CG | MET A 378 | 43.750 | 52.572 | 27.113 | 1.00 | 12.65 | 6 |
| 2974 | CD | PRO A 373 | 46.484 | 67.082 | 26.040 | 1.00 | 13.69 | 6 | 3016 | SD | MET A 378 | 42.871 | 53.357 | 25.713 | 1.00 | 14.01 | 16 |
| 2975 | N | TYR A 374 | 46.374 | 64.933 | 28.815 | 1.00 | 9.68 | 7 | 3017 | CE | MET A 378 | 41.543 | 52.139 | 25.530 | 1.00 | 15.94 | 6 |
| 2976 | CA | TYR A 374 | 47.139 | 63.921 | 29.579 | 1.00 | 10.60 | 6 | 3018 | N | MET A 379 | 42.575 | 53.515 | 30.324 | 1.00 | 11.68 | 7 |
| 2977 | C | TYR A 374 | 46.381 | 63.338 | 30.741 | 1.00 | 11.01 | 6 | 3019 | CA | MET A 379 | 42.364 | 52.843 | 31.637 | 1.00 | 11.67 | 6 |
| 2978 | O | TYR A 374 | 46.896 | 62.356 | 31.346 | 1.00 | 12.41 | 8 | 3020 | C | MET A 379 | 43.364 | 51.711 | 31.705 | 1.00 | 14.11 | 6 |
| 2979 | CB | TYR A 374 | 48.493 | 64.515 | 30.101 | 1.00 | 12.69 | 6 | 3021 | O | MET A 379 | 43.463 | 50.864 | 30.812 | 1.00 | 12.85 | 8 |
| 2980 | CG | TYR A 374 | 49.258 | 65.009 | 28.884 | 1.00 | 14.15 | 6 | 3022 | CB | MET A 379 | 40.896 | 52.323 | 31.558 | 1.00 | 12.77 | 6 |
| 2981 | CD1 | TYR A 374 | 49.738 | 64.107 | 27.954 | 1.00 | 14.25 | 6 | 3023 | CG | MET A 379 | 40.572 | 51.443 | 32.790 | 1.00 | 13.09 | 6 |
| 2982 | CD2 | TYR A 374 | 49.457 | 66.382 | 28.664 | 1.00 | 19.98 | 6 | 3024 | SD | MET A 379 | 40.355 | 52.467 | 34.277 | 1.00 | 13.28 | 16 |
| 2983 | CE1 | TYR A 374 | 50.385 | 64.536 | 26.798 | 1.00 | 19.01 | 6 | 3025 | CE | MET A 379 | 39.369 | 51.269 | 35.254 | 1.00 | 13.26 | 6 |
| 2984 | CE2 | TYR A 374 | 50.125 | 66.791 | 27.525 | 1.00 | 18.34 | 6 | 3026 | N | PRO A 380 | 44.193 | 51.636 | 32.750 | 1.00 | 12.95 | 7 |
| 2985 | CZ | TYR A 374 | 50.572 | 65.893 | 26.613 | 1.00 | 21.81 | 6 | 3027 | CA | PRO A 380 | 45.398 | 50.827 | 32.726 | 1.00 | 14.01 | 6 |
| 2986 | OH | TYR A 374 | 51.271 | 66.349 | 25.492 | 1.00 | 24.57 | 8 | 3028 | C | PRO A 380 | 45.170 | 49.402 | 33.204 | 1.00 | 17.99 | 6 |
| 2987 | N | ASN A 375 | 45.203 | 63.895 | 31.004 | 1.00 | 10.61 | 7 | 3029 | O | PRO A 380 | 46.005 | 48.554 | 32.914 | 1.00 | 17.24 | 8 |
| 2988 | CA | ASN A 375 | 44.295 | 63.320 | 31.991 | 1.00 | 9.59 | 6 | 3030 | CB | PRO A 380 | 46.384 | 51.501 | 33.699 | 1.00 | 14.68 | 6 |
| 2989 | C | ASN A 375 | 43.275 | 62.353 | 31.357 | 1.00 | 11.84 | 6 | 3031 | CG | PRO A 380 | 45.418 | 52.190 | 34.636 | 1.00 | 16.71 | 6 |
| 2990 | O | ASN A 375 | 42.406 | 61.795 | 32.073 | 1.00 | 12.18 | 8 | 3032 | CD | PRO A 380 | 44.300 | 52.693 | 33.751 | 1.00 | 14.00 | 6 |
| 2991 | CB | ASN A 375 | 43.489 | 64.456 | 32.649 | 1.00 | 10.84 | 6 | 3033 | N | ALA A 381 | 44.099 | 49.232 | 33.975 | 1.00 | 15.78 | 7 |
| 2992 | CG | ASN A 375 | 42.822 | 65.356 | 31.632 | 1.00 | 13.47 | 6 | 3034 | CA | ALA A 381 | 43.895 | 47.955 | 34.625 | 1.00 | 13.86 | 6 |
| 2993 | OD1 | ASN A 375 | 42.889 | 65.147 | 30.378 | 1.00 | 14.66 | 8 | 3035 | C | ALA A 381 | 42.477 | 47.891 | 35.190 | 1.00 | 13.98 | 6 |
| 2994 | ND2 | ASN A 375 | 42.188 | 66.403 | 32.155 | 1.00 | 11.13 | 7 | 3036 | O | ALA A 381 | 41.859 | 48.952 | 35.215 | 1.00 | 13.69 | 8 |
| 2995 | N | ARG A 376 | 43.519 | 62.009 | 30.071 | 1.00 | 11.23 | 7 | 3037 | CB | ALA A 381 | 44.854 | 47.608 | 35.761 | 1.00 | 17.52 | 6 |
| 2996 | CA | ARG A 376 | 42.622 | 61.074 | 29.366 | 1.00 | 12.81 | 6 | 3038 | N | PHE A 382 | 42.029 | 46.671 | 35.497 | 1.00 | 14.05 | 7 |
| 2997 | C | ARG A 376 | 43.410 | 59.886 | 28.872 | 1.00 | 11.47 | 6 | 3039 | CA | PHE A 382 | 40.701 | 46.466 | 36.094 | 1.00 | 12.60 | 6 |
| 2998 | O | ARG A 376 | 43.286 | 59.389 | 27.744 | 1.00 | 11.36 | 8 | 3040 | C | PHE A 382 | 40.791 | 45.644 | 37.393 | 1.00 | 12.68 | 6 |
| 2999 | CB | ARG A 376 | 41.975 | 61.789 | 28.128 | 1.00 | 11.93 | 6 | 3041 | O | PHE A 382 | 39.963 | 44.765 | 37.641 | 1.00 | 15.80 | 8 |
| 3000 | CG | ARG A 376 | 41.111 | 62.997 | 28.659 | 1.00 | 11.44 | 6 | 3042 | CB | PHE A 382 | 39.742 | 45.806 | 35.052 | 1.00 | 15.36 | 6 |
| 3001 | CD | ARG A 376 | 40.908 | 63.980 | 27.521 | 1.00 | 13.66 | 6 | 3043 | CG | PHE A 382 | 39.619 | 46.669 | 33.826 | 1.00 | 14.57 | 6 |
| 3002 | NE | ARG A 376 | 40.177 | 65.214 | 28.005 | 1.00 | 13.05 | 7 | 3044 | CD1 | PHE A 382 | 40.475 | 46.629 | 32.737 | 1.00 | 14.43 | 6 |
| 3003 | CZ | ARG A 376 | 39.567 | 66.011 | 27.137 | 1.00 | 11.35 | 6 | 3045 | CD2 | PHE A 382 | 38.572 | 47.618 | 33.775 | 1.00 | 16.09 | 6 |
| 3004 | NH1 | ARG A 376 | 39.569 | 65.752 | 25.825 | 1.00 | 9.57 | 7 | 3046 | CE1 | PHE A 382 | 40.327 | 47.480 | 31.670 | 1.00 | 17.87 | 6 |
| 3005 | NH2 | ARG A 376 | 38.944 | 67.071 | 27.646 | 1.00 | 10.95 | 7 | 3047 | CE2 | PHE A 382 | 38.414 | 48.469 | 32.699 | 1.00 | 12.38 | 6 |
| 3006 | N | GLY A 377 | 44.270 | 59.361 | 29.749 | 1.00 | 9.89 | 7 | 3048 | CZ | PHE A 382 | 39.293 | 48.395 | 31.613 | 1.00 | 15.80 | 6 |
| 3007 | CA | GLY A 377 | 45.084 | 58.173 | 29.407 | 1.00 | 10.61 | 6 | 3049 | N | ASP A 383 | 41.721 | 46.138 | 38.224 | 1.00 | 13.84 | 7 |
| 3008 | C | GLY A 377 | 44.162 | 56.943 | 29.297 | 1.00 | 11.99 | 6 | 3050 | CA | ASP A 383 | 42.065 | 45.402 | 39.467 | 1.00 | 15.38 | 6 |
| 3009 | O | GLY A 377 | 42.974 | 56.949 | 29.658 | 1.00 | 10.52 | 8 | 3051 | C | ASP A 383 | 41.067 | 45.732 | 40.552 | 1.00 | 15.05 | 6 |
| 3010 | N | MET A 378 | 44.783 | 55.861 | 28.718 | 1.00 | 12.46 | 7 | 3052 | O | ASP A 383 | 40.864 | 46.868 | 40.943 | 1.00 | 16.64 | 8 |
| 3011 | CA | MET A 378 | 43.968 | 54.622 | 28.638 | 1.00 | 11.69 | 6 | 3053 | CB | ASP A 383 | 43.457 | 45.826 | 39.901 | 1.00 | 13.18 | 6 |
| 3012 | C | MET A 378 | 43.777 | 54.021 | 30.032 | 1.00 | 11.73 | 6 | 3054 | CG | ASP A 383 | 44.015 | 45.155 | 41.165 | 1.00 | 18.89 | 6 |

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|------|---------------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 3055 | OD1 ASP A 383 | 43.286 | 44.428 | 41.805 | 1.00 | 20.99 | 8 | 3097 | CD2 PHE A 389 | 37.375 | 48.299 | 41.777 | 1.00 | 14.39 | 6 |
| 3056 | OD2 ASP A 383 | 45.229 | 45.408 | 41.363 | 1.00 | 21.43 | 8 | 3098 | CE1 PHE A 389 | 35.869 | 46.515 | 43.383 | 1.00 | 14.50 | 6 |
| 3057 | N THR A 384 | 40.302 | 44.680 | 40.950 | 1.00 | 13.75 | 7 | 3099 | CE2 PHE A 389 | 36.340 | 47.536 | 41.216 | 1.00 | 12.44 | 6 |
| 3058 | CA THR A 384 | 39.215 | 44.894 | 41.930 | 1.00 | 12.49 | 6 | 3100 | CZ PHE A 389 | 35.646 | 46.648 | 42.031 | 1.00 | 13.69 | 6 |
| 3059 | C THR A 384 | 39.773 | 44.871 | 43.345 | 1.00 | 13.78 | 6 | 3101 | N LYS A 390 | 38.053 | 49.160 | 46.775 | 1.00 | 12.03 | 7 |
| 3060 | O THR A 384 | 38.951 | 44.852 | 44.298 | 1.00 | 18.13 | 8 | 3102 | CA LYS A 390 | 37.303 | 48.672 | 47.936 | 1.00 | 12.63 | 6 |
| 3061 | CB THR A 384 | 38.098 | 43.831 | 41.755 | 1.00 | 16.42 | 6 | 3103 | C LYS A 390 | 36.544 | 49.767 | 48.699 | 1.00 | 14.75 | 6 |
| 3062 | OG1 THR A 384 | 38.725 | 42.525 | 41.937 | 1.00 | 18.75 | 8 | 3104 | O LYS A 390 | 35.438 | 49.556 | 48.197 | 1.00 | 12.66 | 8 |
| 3063 | CG2 THR A 384 | 37.515 | 43.943 | 40.342 | 1.00 | 20.28 | 6 | 3105 | CB LYS A 390 | 38.291 | 48.000 | 49.197 | 1.00 | 12.06 | 6 |
| 3064 | N THR A 385 | 41.088 | 44.832 | 43.573 | 1.00 | 14.37 | 7 | 3106 | CG LYS A 390 | 38.798 | 46.712 | 48.243 | 1.00 | 15.90 | 6 |
| 3065 | CA THR A 385 | 41.648 | 44.691 | 44.906 | 1.00 | 16.71 | 6 | 3107 | CD LYS A 390 | 39.589 | 45.970 | 49.325 | 1.00 | 25.81 | 6 |
| 3066 | C THR A 385 | 42.313 | 45.974 | 45.424 | 1.00 | 16.63 | 6 | 3108 | CE LYS A 390 | 40.980 | 46.524 | 49.440 | 1.00 | 29.79 | 6 |
| 3067 | O THR A 385 | 42.873 | 45.952 | 46.539 | 1.00 | 14.22 | 8 | 3109 | NZ LYS A 390 | 41.835 | 45.465 | 50.107 | 1.00 | 41.01 | 7 |
| 3068 | CB THR A 385 | 42.693 | 43.546 | 45.009 | 1.00 | 19.15 | 6 | 3110 | N GLU A 391 | 37.256 | 50.908 | 48.782 | 1.00 | 11.21 | 7 |
| 3069 | OG1 THR A 385 | 43.883 | 43.878 | 44.288 | 1.00 | 17.99 | 8 | 3111 | CA GLU A 391 | 36.636 | 52.048 | 49.475 | 1.00 | 11.43 | 6 |
| 3070 | CG2 THR A 385 | 42.075 | 42.234 | 44.541 | 1.00 | 24.33 | 6 | 3112 | C GLU A 391 | 35.375 | 52.482 | 48.742 | 1.00 | 12.51 | 6 |
| 3071 | N THR A 386 | 42.254 | 47.039 | 44.506 | 1.00 | 14.92 | 7 | 3113 | O GLU A 391 | 34.300 | 52.735 | 49.337 | 1.00 | 10.64 | 8 |
| 3072 | CA THR A 386 | 42.952 | 48.254 | 45.131 | 1.00 | 13.63 | 6 | 3114 | CB GLU A 391 | 37.670 | 53.223 | 49.487 | 1.00 | 10.44 | 6 |
| 3073 | C THR A 386 | 42.175 | 48.801 | 46.328 | 1.00 | 11.22 | 6 | 3115 | CG GLU A 391 | 36.957 | 54.519 | 49.997 | 1.00 | 10.67 | 6 |
| 3074 | O THR A 386 | 40.990 | 48.649 | 46.478 | 1.00 | 12.74 | 8 | 3116 | CD GLU A 391 | 37.870 | 55.744 | 49.810 | 1.00 | 12.38 | 6 |
| 3075 | CB THR A 386 | 43.101 | 49.344 | 44.054 | 1.00 | 13.50 | 6 | 3117 | OE1 GLU A 391 | 38.974 | 55.628 | 49.226 | 1.00 | 13.12 | 8 |
| 3076 | OG1 THR A 386 | 41.805 | 49.919 | 43.822 | 1.00 | 12.14 | 8 | 3118 | OE2 GLU A 391 | 37.458 | 56.841 | 50.284 | 1.00 | 12.94 | 8 |
| 3077 | CG2 THR A 386 | 43.656 | 48.809 | 42.719 | 1.00 | 17.62 | 6 | 3119 | N VAL A 392 | 35.455 | 52.675 | 47.403 | 1.00 | 11.36 | 7 |
| 3078 | N THR A 387 | 42.886 | 49.552 | 47.184 | 1.00 | 14.21 | 7 | 3120 | CA VAL A 392 | 34.279 | 53.176 | 46.653 | 1.00 | 12.25 | 6 |
| 3079 | CA THR A 387 | 42.237 | 50.167 | 48.316 | 1.00 | 11.44 | 6 | 3121 | C VAL A 392 | 33.156 | 52.128 | 46.716 | 1.00 | 12.76 | 6 |
| 3080 | C THR A 387 | 41.127 | 51.134 | 47.887 | 1.00 | 12.54 | 6 | 3122 | O VAL A 392 | 31.968 | 52.481 | 46.930 | 1.00 | 12.77 | 8 |
| 3081 | O THR A 387 | 40.045 | 51.113 | 48.437 | 1.00 | 12.57 | 8 | 3123 | CB VAL A 392 | 34.667 | 53.410 | 45.175 | 1.00 | 14.39 | 6 |
| 3082 | CB THR A 387 | 43.277 | 50.926 | 49.145 | 1.00 | 17.16 | 6 | 3124 | CG1 VAL A 392 | 33.434 | 53.661 | 44.296 | 1.00 | 13.75 | 6 |
| 3083 | OG1 THR A 387 | 44.177 | 49.939 | 49.669 | 1.00 | 15.42 | 8 | 3125 | CG2 VAL A 392 | 35.702 | 54.570 | 45.061 | 1.00 | 12.07 | 6 |
| 3084 | CG2 THR A 387 | 42.644 | 51.724 | 50.273 | 1.00 | 14.27 | 6 | 3126 | N SER A 393 | 33.487 | 50.846 | 46.628 | 1.00 | 10.90 | 7 |
| 3085 | N ALA A 388 | 41.441 | 51.910 | 46.838 | 1.00 | 13.30 | 7 | 3127 | CA SER A 393 | 32.426 | 49.822 | 46.686 | 1.00 | 12.19 | 6 |
| 3086 | CA ALA A 388 | 40.376 | 52.785 | 46.360 | 1.00 | 10.83 | 6 | 3128 | C SER A 393 | 31.708 | 49.782 | 48.021 | 1.00 | 10.96 | 6 |
| 3087 | O ALA A 388 | 39.162 | 52.083 | 45.808 | 1.00 | 12.23 | 6 | 3129 | O SER A 393 | 30.469 | 49.774 | 48.186 | 1.00 | 12.48 | 8 |
| 3088 | O ALA A 388 | 38.030 | 52.497 | 46.001 | 1.00 | 11.44 | 8 | 3130 | CB SER A 393 | 33.059 | 48.431 | 46.394 | 1.00 | 12.79 | 6 |
| 3089 | CB ALA A 388 | 40.968 | 53.700 | 45.239 | 1.00 | 10.26 | 6 | 3131 | OG SER A 393 | 31.944 | 47.538 | 46.423 | 1.00 | 19.93 | 8 |
| 3090 | N PHE A 389 | 39.347 | 50.956 | 45.084 | 1.00 | 12.53 | 7 | 3132 | N THR A 394 | 32.493 | 49.942 | 49.099 | 1.00 | 11.04 | 7 |
| 3091 | CA PHE A 389 | 38.202 | 50.182 | 44.579 | 1.00 | 13.64 | 6 | 3133 | CA THR A 394 | 31.920 | 49.922 | 50.445 | 1.00 | 12.34 | 6 |
| 3092 | C PHE A 389 | 37.361 | 49.746 | 45.779 | 1.00 | 13.47 | 6 | 3134 | C THR A 394 | 31.061 | 51.130 | 50.682 | 1.00 | 11.80 | 6 |
| 3093 | O PHE A 389 | 36.157 | 49.895 | 45.789 | 1.00 | 12.37 | 8 | 3135 | O THR A 394 | 29.935 | 51.097 | 51.169 | 1.00 | 11.63 | 8 |
| 3094 | CB PHE A 389 | 38.766 | 48.975 | 43.763 | 1.00 | 11.46 | 6 | 3136 | CB THR A 394 | 33.039 | 49.889 | 51.509 | 1.00 | 12.40 | 6 |
| 3095 | OG PHE A 389 | 37.627 | 48.178 | 43.141 | 1.00 | 12.01 | 6 | 3137 | OG1 THR A 394 | 33.699 | 48.614 | 51.401 | 1.00 | 14.67 | 8 |
| 3096 | CD1 PHE A 389 | 36.936 | 47.248 | 43.916 | 1.00 | 16.87 | 6 | 3138 | CG2 THR A 394 | 32.443 | 50.011 | 52.927 | 1.00 | 14.84 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3139 | N | LEU A 395 | 31.600 | 52.334 | 50.322 | 1.00 | 12.76 | 7 | 3181 | CD | ARG A 400 | 23.412 | 50.634 | 45.761 | 1.00 | 16.08 | 6 |
| 3140 | CA | LEU A 395 | 30.858 | 53.558 | 50.592 | 1.00 | 11.35 | 6 | 3182 | NE | ARG A 400 | 24.141 | 49.517 | 46.399 | 1.00 | 14.78 | 7 |
| 3141 | C | LEU A 395 | 29.666 | 53.709 | 49.624 | 1.00 | 10.18 | 6 | 3183 | CZ | ARG A 400 | 25.452 | 49.279 | 46.343 | 1.00 | 14.12 | 6 |
| 3142 | O | LEU A 395 | 28.676 | 54.373 | 49.976 | 1.00 | 11.69 | 8 | 3184 | NH1 | ARG A 400 | 26.214 | 50.128 | 45.640 | 1.00 | 15.84 | 7 |
| 3143 | CB | LEU A 395 | 31.784 | 54.804 | 50.604 | 1.00 | 13.30 | 6 | 3185 | NH2 | ARG A 400 | 25.957 | 48.216 | 46.978 | 1.00 | 16.89 | 7 |
| 3144 | CG | LEU A 395 | 32.795 | 54.745 | 51.811 | 1.00 | 12.96 | 6 | 3186 | N | ASN A 401 | 22.154 | 52.394 | 50.972 | 1.00 | 14.24 | 7 |
| 3145 | CD1 | LEU A 395 | 33.641 | 56.019 | 51.748 | 1.00 | 13.55 | 6 | 3187 | CA | ASN A 401 | 21.271 | 51.879 | 52.060 | 1.00 | 14.18 | 6 |
| 3146 | CD2 | LEU A 395 | 32.059 | 54.747 | 53.145 | 1.00 | 14.45 | 6 | 3188 | C | ASN A 401 | 20.967 | 52.828 | 53.189 | 1.00 | 15.56 | 6 |
| 3147 | N | ALA A 396 | 29.852 | 53.116 | 48.444 | 1.00 | 11.70 | 7 | 3189 | O | ASN A 401 | 19.976 | 52.564 | 53.935 | 1.00 | 17.91 | 8 |
| 3148 | CA | ALA A 396 | 28.636 | 53.182 | 47.557 | 1.00 | 12.78 | 6 | 3190 | CB | ASN A 401 | 21.990 | 50.632 | 52.590 | 1.00 | 16.43 | 6 |
| 3149 | C | ALA A 396 | 27.498 | 52.378 | 48.163 | 1.00 | 13.72 | 6 | 3191 | CG | ASN A 401 | 21.827 | 49.617 | 51.404 | 1.00 | 25.29 | 6 |
| 3150 | O | ALA A 396 | 26.345 | 52.797 | 48.075 | 1.00 | 10.99 | 8 | 3192 | OD1 | ASN A 401 | 22.805 | 49.256 | 50.797 | 1.00 | 33.03 | 8 |
| 3151 | CB | ALA A 396 | 29.035 | 52.530 | 46.203 | 1.00 | 12.34 | 6 | 3193 | ND2 | ASN A 401 | 20.619 | 49.215 | 51.102 | 1.00 | 40.20 | 7 |
| 3152 | N | GLY A 397 | 27.797 | 51.244 | 48.825 | 1.00 | 11.86 | 7 | 3194 | N | ASN A 402 | 21.705 | 53.948 | 53.373 | 1.00 | 13.76 | 7 |
| 3153 | CA | GLY A 397 | 26.710 | 50.490 | 49.510 | 1.00 | 12.95 | 6 | 3195 | CA | ASN A 402 | 21.449 | 54.851 | 54.506 | 1.00 | 13.71 | 6 |
| 3154 | C | GLY A 397 | 26.096 | 51.295 | 50.556 | 1.00 | 12.93 | 6 | 3196 | C | ASN A 402 | 20.938 | 56.175 | 53.980 | 1.00 | 14.67 | 6 |
| 3155 | O | GLY A 397 | 24.865 | 51.276 | 50.842 | 1.00 | 15.22 | 8 | 3197 | O | ASN A 402 | 21.601 | 56.923 | 53.249 | 1.00 | 13.53 | 8 |
| 3156 | N | LEU A 398 | 26.948 | 52.018 | 51.404 | 1.00 | 12.12 | 7 | 3198 | CB | ASN A 402 | 22.753 | 55.036 | 55.311 | 1.00 | 13.24 | 6 |
| 3157 | CA | LEU A 398 | 26.336 | 52.833 | 52.491 | 1.00 | 10.40 | 6 | 3199 | CG | ASN A 402 | 22.397 | 55.744 | 56.604 | 1.00 | 14.53 | 6 |
| 3158 | C | LEU A 398 | 25.388 | 53.871 | 51.900 | 1.00 | 13.47 | 6 | 3200 | OD1 | ASN A 402 | 21.722 | 56.787 | 56.564 | 1.00 | 14.56 | 8 |
| 3159 | O | LEU A 398 | 24.310 | 54.166 | 52.434 | 1.00 | 13.29 | 8 | 3201 | ND2 | ASN A 402 | 22.839 | 55.186 | 57.762 | 1.00 | 11.48 | 7 |
| 3160 | CB | LEU A 398 | 27.503 | 53.525 | 53.229 | 1.00 | 10.78 | 6 | 3202 | N | ALA A 403 | 19.633 | 56.460 | 54.202 | 1.00 | 12.55 | 7 |
| 3161 | CG | LEU A 398 | 26.999 | 54.426 | 54.353 | 1.00 | 11.76 | 6 | 3203 | CA | ALA A 403 | 19.017 | 57.672 | 53.679 | 1.00 | 12.81 | 6 |
| 3162 | CD1 | LEU A 398 | 26.326 | 53.660 | 55.479 | 1.00 | 15.25 | 6 | 3204 | C | ALA A 403 | 19.622 | 58.961 | 54.144 | 1.00 | 14.88 | 6 |
| 3163 | CD2 | LEU A 398 | 28.230 | 55.206 | 54.909 | 1.00 | 16.57 | 6 | 3205 | O | ALA A 403 | 19.421 | 59.958 | 53.422 | 1.00 | 13.18 | 8 |
| 3164 | N | ARG A 399 | 25.832 | 54.478 | 50.754 | 1.00 | 11.98 | 7 | 3206 | CB | ALA A 403 | 17.511 | 57.608 | 54.092 | 1.00 | 12.99 | 6 |
| 3165 | CA | ARG A 399 | 24.988 | 55.539 | 50.164 | 1.00 | 12.52 | 6 | 3207 | N | ALA A 404 | 20.407 | 58.945 | 55.229 | 1.00 | 11.82 | 7 |
| 3166 | C | ARG A 399 | 23.712 | 54.952 | 49.579 | 1.00 | 13.24 | 6 | 3208 | CA | ALA A 404 | 21.107 | 60.187 | 55.611 | 1.00 | 11.98 | 6 |
| 3167 | O | ARG A 399 | 22.661 | 55.603 | 49.588 | 1.00 | 14.42 | 8 | 3209 | C | ALA A 404 | 22.095 | 60.641 | 54.524 | 1.00 | 11.49 | 6 |
| 3168 | CB | ARG A 399 | 25.789 | 56.271 | 49.068 | 1.00 | 11.24 | 6 | 3210 | O | ALA A 404 | 22.259 | 61.857 | 54.383 | 1.00 | 12.58 | 8 |
| 3169 | CG | ARG A 399 | 24.974 | 57.205 | 48.158 | 1.00 | 11.40 | 6 | 3211 | CB | ALA A 404 | 21.874 | 60.008 | 56.930 | 1.00 | 15.02 | 6 |
| 3170 | CD | ARG A 399 | 25.933 | 57.875 | 47.182 | 1.00 | 11.42 | 6 | 3212 | N | ILE A 405 | 22.707 | 59.716 | 53.830 | 1.00 | 11.27 | 7 |
| 3171 | NE | ARG A 399 | 26.620 | 59.029 | 47.799 | 1.00 | 10.92 | 7 | 3213 | CA | ILE A 405 | 23.702 | 60.168 | 52.791 | 1.00 | 11.62 | 6 |
| 3172 | CZ | ARG A 399 | 26.193 | 60.279 | 47.877 | 1.00 | 14.21 | 6 | 3214 | C | ILE A 405 | 22.936 | 60.722 | 51.581 | 1.00 | 13.21 | 6 |
| 3173 | NH1 | ARG A 399 | 24.965 | 60.565 | 47.446 | 1.00 | 10.96 | 7 | 3215 | O | ILE A 405 | 23.353 | 61.696 | 50.964 | 1.00 | 12.14 | 8 |
| 3174 | NH2 | ARG A 399 | 26.954 | 61.245 | 48.436 | 1.00 | 11.76 | 7 | 3216 | CB | ILE A 405 | 24.538 | 58.973 | 52.331 | 1.00 | 14.54 | 6 |
| 3175 | N | ARG A 400 | 23.713 | 53.697 | 49.131 | 1.00 | 12.24 | 7 | 3217 | CG1 | ILE A 405 | 25.425 | 58.253 | 53.392 | 1.00 | 15.40 | 6 |
| 3176 | CA | ARG A 400 | 22.456 | 53.111 | 48.675 | 1.00 | 12.96 | 6 | 3218 | CG2 | ILE A 405 | 25.511 | 59.410 | 51.202 | 1.00 | 11.30 | 6 |
| 3177 | C | ARG A 400 | 21.533 | 52.789 | 49.852 | 1.00 | 13.71 | 6 | 3219 | CD1 | ILE A 405 | 26.170 | 59.266 | 54.247 | 1.00 | 17.36 | 6 |
| 3178 | O | ARG A 400 | 20.311 | 52.762 | 49.629 | 1.00 | 17.33 | 8 | 3220 | N | GLN A 406 | 21.759 | 60.152 | 51.297 | 1.00 | 11.32 | 7 |
| 3179 | CB | ARG A 400 | 22.748 | 51.783 | 47.930 | 1.00 | 14.09 | 6 | 3221 | CA | GLN A 406 | 20.992 | 60.545 | 50.107 | 1.00 | 11.87 | 6 |
| 3180 | CG | ARG A 400 | 23.460 | 51.918 | 46.578 | 1.00 | 14.91 | 6 | 3222 | C | GLN A 406 | 20.335 | 61.902 | 50.300 | 1.00 | 14.28 | 6 |

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|------|-----|-----------|--------|--------|--------|------------|---|------|---------------|--------|--------|--------|------------|---|
| 3223 | O | GLN A 406 | 20.265 | 62.707 | 49.360 | 1.00 11.82 | 8 | 3265 | CG2 THR A 411 | 25.620 | 69.676 | 62.991 | 1.00 17.79 | 6 |
| 3224 | CB | GLN A 406 | 19.875 | 59.494 | 49.869 | 1.00 12.00 | 6 | 3266 | N GLN A 412 | 28.501 | 70.302 | 61.110 | 1.00 12.74 | 7 |
| 3225 | CG | GLN A 406 | 20.511 | 58.136 | 49.549 | 1.00 12.17 | 6 | 3267 | CA GLN A 412 | 29.899 | 70.153 | 61.592 | 1.00 13.61 | 6 |
| 3226 | CG | GLN A 406 | 19.521 | 56.983 | 49.392 | 1.00 22.22 | 6 | 3268 | C GLN A 412 | 29.894 | 69.765 | 63.062 | 1.00 13.43 | 6 |
| 3227 | OE1 | GLN A 406 | 19.847 | 55.775 | 49.395 | 1.00 20.31 | 8 | 3269 | O GLN A 412 | 29.218 | 70.451 | 63.824 | 1.00 15.64 | 8 |
| 3228 | NE2 | GLN A 406 | 18.272 | 57.356 | 49.223 | 1.00 24.04 | 7 | 3270 | GLN A 412 | 30.556 | 71.523 | 61.335 | 1.00 14.70 | 6 |
| 3229 | N | TYR A 407 | 19.757 | 62.154 | 51.499 | 1.00 13.05 | 7 | 3271 | CG GLN A 412 | 31.999 | 71.615 | 61.876 | 1.00 22.99 | 6 |
| 3230 | CA | TYR A 407 | 18.848 | 63.261 | 51.702 | 1.00 13.56 | 6 | 3272 | CD GLN A 412 | 31.918 | 72.168 | 63.334 | 1.00 22.07 | 6 |
| 3231 | C | TYR A 407 | 19.168 | 64.182 | 52.885 | 1.00 10.35 | 6 | 3273 | OE1 GLN A 412 | 32.409 | 71.438 | 64.163 | 1.00 19.41 | 8 |
| 3232 | O | TYR A 407 | 18.463 | 65.190 | 53.047 | 1.00 12.85 | 8 | 3274 | NE2 GLN A 412 | 31.358 | 73.310 | 63.633 | 1.00 25.10 | 7 |
| 3233 | CB | TYR A 407 | 17.440 | 62.678 | 52.068 | 1.00 14.06 | 6 | 3275 | N ARG A 413 | 30.694 | 68.721 | 63.330 | 1.00 11.94 | 7 |
| 3234 | CG | TYR A 407 | 16.935 | 61.567 | 51.144 | 1.00 12.51 | 6 | 3276 | CA ARG A 413 | 30.768 | 68.223 | 64.700 | 1.00 11.40 | 6 |
| 3235 | CD1 | TYR A 407 | 16.929 | 61.748 | 49.759 | 1.00 11.68 | 6 | 3277 | C ARG A 413 | 32.184 | 68.430 | 65.276 | 1.00 12.19 | 6 |
| 3236 | CD2 | TYR A 407 | 16.397 | 60.418 | 51.708 | 1.00 11.57 | 6 | 3278 | O ARG A 413 | 32.263 | 68.482 | 66.510 | 1.00 12.20 | 8 |
| 3237 | CE1 | TYR A 407 | 16.441 | 60.742 | 48.918 | 1.00 12.71 | 6 | 3279 | CB ARG A 413 | 30.356 | 66.756 | 64.815 | 1.00 16.20 | 6 |
| 3238 | CE2 | TYR A 407 | 15.910 | 59.420 | 50.894 | 1.00 14.60 | 6 | 3280 | CG ARG A 413 | 28.840 | 66.557 | 64.562 | 1.00 13.09 | 6 |
| 3239 | CZ | TYR A 407 | 15.933 | 59.595 | 49.515 | 1.00 15.50 | 6 | 3281 | CD ARG A 413 | 27.968 | 67.296 | 65.579 | 1.00 13.13 | 6 |
| 3240 | OH | TYR A 407 | 15.433 | 58.598 | 48.707 | 1.00 15.89 | 8 | 3282 | NE ARG A 413 | 26.611 | 66.668 | 65.580 | 1.00 14.79 | 7 |
| 3241 | N | GLY A 408 | 20.152 | 63.743 | 53.678 | 1.00 12.31 | 7 | 3283 | CZ ARG A 413 | 25.684 | 66.909 | 66.515 | 1.00 19.43 | 6 |
| 3242 | CA | GLY A 408 | 20.277 | 64.361 | 55.005 | 1.00 14.17 | 6 | 3284 | NH1 ARG A 413 | 25.974 | 67.784 | 67.503 | 1.00 16.73 | 7 |
| 3243 | C | GLY A 408 | 20.830 | 65.790 | 55.030 | 1.00 13.76 | 6 | 3285 | NH2 ARG A 413 | 24.529 | 66.233 | 66.470 | 1.00 18.22 | 7 |
| 3244 | O | GLY A 408 | 21.566 | 66.253 | 54.133 | 1.00 13.31 | 8 | 3286 | N TRP A 414 | 33.228 | 68.466 | 64.474 | 1.00 11.18 | 7 |
| 3245 | CA | THR A 409 | 20.636 | 66.393 | 56.207 | 1.00 12.33 | 7 | 3287 | CA TRP A 414 | 34.548 | 68.752 | 65.082 | 1.00 12.61 | 6 |
| 3246 | CA | THR A 409 | 21.322 | 67.645 | 56.558 | 1.00 14.50 | 6 | 3288 | C TRP A 414 | 35.444 | 69.243 | 63.947 | 1.00 13.80 | 6 |
| 3247 | C | THR A 409 | 22.822 | 67.370 | 56.707 | 1.00 13.72 | 6 | 3289 | O TRP A 414 | 35.295 | 68.712 | 62.833 | 1.00 13.58 | 8 |
| 3248 | O | THR A 409 | 23.222 | 66.229 | 56.777 | 1.00 12.71 | 8 | 3290 | CB TRP A 414 | 35.121 | 67.438 | 65.651 | 1.00 14.04 | 6 |
| 3249 | CB | THR A 409 | 20.812 | 68.210 | 57.928 | 1.00 16.13 | 6 | 3291 | CG TRP A 414 | 36.181 | 67.603 | 66.709 | 1.00 14.49 | 6 |
| 3250 | OG1 | THR A 409 | 20.849 | 67.169 | 58.916 | 1.00 16.69 | 8 | 3292 | CD1 TRP A 414 | 35.921 | 67.473 | 68.075 | 1.00 15.45 | 6 |
| 3251 | CG2 | THR A 409 | 19.360 | 68.677 | 57.762 | 1.00 18.70 | 6 | 3293 | CD2 TRP A 414 | 37.583 | 67.864 | 66.591 | 1.00 15.74 | 6 |
| 3252 | N | THR A 410 | 23.605 | 68.449 | 56.790 | 1.00 12.28 | 7 | 3294 | NE1 TRP A 414 | 37.112 | 67.622 | 68.773 | 1.00 16.17 | 7 |
| 3253 | CA | THR A 410 | 25.062 | 68.261 | 57.141 | 1.00 12.15 | 6 | 3295 | CE2 TRP A 414 | 38.123 | 67.884 | 67.898 | 1.00 15.43 | 6 |
| 3254 | C | THR A 410 | 25.332 | 69.229 | 58.321 | 1.00 12.71 | 6 | 3296 | CE3 TRP A 414 | 38.421 | 68.101 | 65.507 | 1.00 14.89 | 6 |
| 3255 | O | THR A 410 | 25.041 | 70.423 | 58.225 | 1.00 13.99 | 8 | 3297 | CZ2 TRP A 414 | 39.489 | 68.090 | 68.138 | 1.00 20.21 | 6 |
| 3256 | CB | THR A 410 | 25.943 | 68.740 | 55.952 | 1.00 11.34 | 6 | 3298 | CZ3 TRP A 414 | 39.805 | 68.279 | 65.725 | 1.00 15.42 | 6 |
| 3257 | OG1 | THR A 410 | 25.541 | 67.959 | 54.786 | 1.00 13.77 | 8 | 3299 | CH2 TRP A 414 | 40.310 | 68.296 | 67.066 | 1.00 17.01 | 6 |
| 3258 | CG2 | THR A 410 | 27.425 | 68.392 | 56.192 | 1.00 13.33 | 6 | 3300 | N ILE A 415 | 36.215 | 70.337 | 64.186 | 1.00 12.40 | 7 |
| 3259 | N | THR A 411 | 25.996 | 68.665 | 59.342 | 1.00 12.78 | 7 | 3301 | CA ILE A 415 | 37.012 | 70.828 | 63.038 | 1.00 11.33 | 6 |
| 3260 | CA | THR A 411 | 26.301 | 69.430 | 60.568 | 1.00 12.27 | 6 | 3302 | C ILE A 415 | 38.296 | 71.491 | 63.524 | 1.00 15.04 | 6 |
| 3261 | C | THR A 411 | 27.765 | 69.192 | 60.919 | 1.00 13.51 | 6 | 3303 | O ILE A 415 | 38.300 | 72.134 | 64.600 | 1.00 15.39 | 8 |
| 3262 | O | THR A 411 | 28.168 | 68.039 | 61.036 | 1.00 14.10 | 8 | 3304 | CB ILE A 415 | 36.153 | 71.827 | 62.253 | 1.00 15.29 | 6 |
| 3263 | CB | THR A 411 | 25.386 | 68.891 | 61.718 | 1.00 13.83 | 6 | 3305 | CG1 ILE A 415 | 36.843 | 72.197 | 60.923 | 1.00 15.07 | 6 |
| 3264 | OG1 | THR A 411 | 24.000 | 69.120 | 61.364 | 1.00 15.26 | 8 | 3306 | CG2 ILE A 415 | 35.782 | 73.061 | 63.054 | 1.00 20.69 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3307 | CD1 | ILE A 415 | 35.862 | 72.686 | 59.854 | 1.00 | 18.18 | 6 | 3349 | CZ | TYR A 420 | 32.692 | 69.780 | 57.021 | 1.00 | 15.49 | 6 |
| 3308 | N | ASN A 416 | 39.349 | 71.266 | 62.797 | 1.00 | 13.47 | 7 | 3350 | OH | TYR A 420 | 31.503 | 70.412 | 56.683 | 1.00 | 15.26 | 8 |
| 3309 | CA | ASN A 416 | 40.517 | 72.152 | 62.912 | 1.00 | 14.63 | 6 | 3351 | N | ILE A 421 | 35.000 | 66.508 | 61.075 | 1.00 | 11.61 | 7 |
| 3310 | C | ASN A 416 | 41.103 | 72.198 | 61.526 | 1.00 | 13.17 | 6 | 3352 | CA | ILE A 421 | 34.037 | 65.462 | 61.458 | 1.00 | 9.13 | 6 |
| 3311 | O | ASN A 416 | 40.399 | 71.879 | 60.536 | 1.00 | 12.76 | 8 | 3353 | C | ILE A 421 | 32.649 | 66.076 | 61.282 | 1.00 | 10.90 | 6 |
| 3312 | CB | ASN A 416 | 41.480 | 71.607 | 63.994 | 1.00 | 14.61 | 6 | 3354 | O | ILE A 421 | 32.379 | 67.148 | 61.788 | 1.00 | 13.13 | 8 |
| 3313 | CG | ASN A 416 | 42.250 | 70.394 | 63.669 | 1.00 | 16.07 | 6 | 3355 | CB | ILE A 421 | 34.238 | 64.997 | 62.941 | 1.00 | 11.03 | 6 |
| 3314 | OD1 | ASN A 416 | 42.180 | 69.778 | 62.591 | 1.00 | 12.99 | 8 | 3356 | CG1 | ILE A 421 | 35.689 | 64.584 | 63.133 | 1.00 | 11.76 | 6 |
| 3315 | ND2 | ASN A 416 | 43.129 | 69.947 | 64.597 | 1.00 | 16.12 | 7 | 3357 | CG2 | ILE A 421 | 33.251 | 63.841 | 63.198 | 1.00 | 14.22 | 6 |
| 3316 | N | ASN A 417 | 42.356 | 72.644 | 61.313 | 1.00 | 13.23 | 7 | 3358 | CD1 | ILE A 421 | 35.980 | 63.871 | 64.484 | 1.00 | 14.70 | 6 |
| 3317 | CA | ASN A 417 | 42.755 | 72.836 | 59.907 | 1.00 | 13.30 | 6 | 3359 | N | TYR A 422 | 31.889 | 65.498 | 60.276 | 1.00 | 10.51 | 7 |
| 3318 | C | ASN A 417 | 42.767 | 71.526 | 59.103 | 1.00 | 13.34 | 6 | 3360 | CA | TYR A 422 | 30.571 | 66.072 | 60.004 | 1.00 | 11.77 | 6 |
| 3319 | O | ASN A 417 | 42.621 | 71.524 | 57.886 | 1.00 | 12.55 | 8 | 3361 | C | TYR A 422 | 29.510 | 64.963 | 60.053 | 1.00 | 11.33 | 6 |
| 3320 | CB | ASN A 417 | 44.185 | 73.410 | 59.931 | 1.00 | 16.87 | 6 | 3362 | O | TYR A 422 | 29.877 | 63.774 | 59.986 | 1.00 | 11.55 | 8 |
| 3321 | CG | ASN A 417 | 44.190 | 74.929 | 59.999 | 1.00 | 23.81 | 6 | 3363 | CB | TYR A 422 | 30.570 | 66.791 | 58.623 | 1.00 | 11.55 | 6 |
| 3322 | OD1 | ASN A 417 | 43.170 | 75.585 | 60.178 | 1.00 | 21.65 | 8 | 3364 | CG | TYR A 422 | 31.000 | 65.881 | 57.458 | 1.00 | 12.40 | 6 |
| 3323 | ND2 | ASN A 417 | 45.415 | 75.482 | 59.839 | 1.00 | 24.48 | 7 | 3365 | CD1 | TYR A 422 | 30.094 | 65.103 | 56.724 | 1.00 | 11.81 | 6 |
| 3324 | N | ASP A 418 | 43.109 | 70.439 | 59.874 | 1.00 | 12.62 | 7 | 3366 | CD2 | TYR A 422 | 32.354 | 65.851 | 57.140 | 1.00 | 11.72 | 6 |
| 3325 | CA | ASP A 418 | 43.295 | 69.150 | 59.209 | 1.00 | 10.76 | 6 | 3367 | CE1 | TYR A 422 | 30.559 | 64.305 | 55.668 | 1.00 | 12.09 | 6 |
| 3326 | C | ASP A 418 | 42.126 | 68.157 | 59.319 | 1.00 | 12.08 | 6 | 3368 | CE2 | TYR A 422 | 32.853 | 65.051 | 56.094 | 1.00 | 11.73 | 6 |
| 3327 | O | ASP A 418 | 42.093 | 67.177 | 58.533 | 1.00 | 11.98 | 8 | 3369 | CZ | TYR A 422 | 31.935 | 64.298 | 55.377 | 1.00 | 13.04 | 6 |
| 3328 | CB | ASP A 418 | 44.520 | 68.478 | 59.846 | 1.00 | 13.38 | 6 | 3370 | OH | TYR A 422 | 32.365 | 63.520 | 54.338 | 1.00 | 11.43 | 8 |
| 3329 | CG | ASP A 418 | 45.842 | 69.080 | 59.483 | 1.00 | 16.78 | 6 | 3371 | N | GLU A 423 | 28.257 | 65.380 | 60.139 | 1.00 | 11.98 | 7 |
| 3330 | OD1 | ASP A 418 | 46.040 | 69.609 | 58.372 | 1.00 | 13.55 | 8 | 3372 | CA | GLU A 423 | 27.202 | 64.378 | 60.362 | 1.00 | 11.04 | 6 |
| 3331 | OD2 | ASP A 418 | 46.759 | 69.017 | 60.342 | 1.00 | 13.98 | 8 | 3373 | C | GLU A 423 | 26.064 | 64.598 | 59.383 | 1.00 | 11.74 | 6 |
| 3332 | N | VAL A 419 | 41.304 | 68.369 | 60.363 | 1.00 | 11.52 | 7 | 3374 | O | GLU A 423 | 25.644 | 65.748 | 59.205 | 1.00 | 13.56 | 8 |
| 3333 | CA | VAL A 419 | 40.281 | 67.366 | 60.644 | 1.00 | 10.52 | 6 | 3375 | CB | GLU A 423 | 26.633 | 64.609 | 61.806 | 1.00 | 14.91 | 6 |
| 3334 | C | VAL A 419 | 38.910 | 67.958 | 60.419 | 1.00 | 12.12 | 6 | 3376 | CG | GLU A 423 | 25.731 | 63.465 | 62.258 | 1.00 | 12.27 | 6 |
| 3335 | O | VAL A 419 | 38.606 | 69.052 | 60.846 | 1.00 | 12.25 | 8 | 3377 | CD | GLU A 423 | 25.459 | 63.688 | 63.796 | 1.00 | 13.28 | 6 |
| 3336 | CB | VAL A 419 | 40.384 | 66.958 | 62.145 | 1.00 | 11.46 | 6 | 3378 | OE1 | GLU A 423 | 24.947 | 64.750 | 64.099 | 1.00 | 18.28 | 8 |
| 3337 | CG1 | VAL A 419 | 39.231 | 65.959 | 62.481 | 1.00 | 11.88 | 6 | 3379 | OE2 | GLU A 423 | 25.800 | 62.682 | 64.408 | 1.00 | 17.49 | 8 |
| 3338 | CG2 | VAL A 419 | 41.737 | 66.266 | 62.444 | 1.00 | 12.56 | 6 | 3380 | N | ARG A 424 | 25.648 | 63.541 | 58.699 | 1.00 | 12.31 | 7 |
| 3339 | N | TYR A 420 | 38.034 | 67.172 | 59.764 | 1.00 | 11.92 | 7 | 3381 | CA | ARG A 424 | 24.457 | 63.621 | 57.847 | 1.00 | 11.64 | 6 |
| 3340 | CA | TYR A 420 | 36.628 | 67.548 | 59.636 | 1.00 | 10.72 | 6 | 3382 | C | ARG A 424 | 23.268 | 63.035 | 58.643 | 1.00 | 13.19 | 6 |
| 3341 | C | TYR A 420 | 35.772 | 66.328 | 59.977 | 1.00 | 10.50 | 6 | 3383 | O | ARG A 424 | 23.515 | 62.077 | 59.367 | 1.00 | 13.04 | 8 |
| 3342 | O | TYR A 420 | 35.908 | 65.254 | 59.363 | 1.00 | 13.20 | 8 | 3384 | CB | ARG A 424 | 24.665 | 62.689 | 56.620 | 1.00 | 10.72 | 6 |
| 3343 | CB | TYR A 420 | 36.410 | 67.866 | 58.138 | 1.00 | 9.44 | 6 | 3385 | CG | ARG A 424 | 25.961 | 63.049 | 55.805 | 1.00 | 10.81 | 6 |
| 3344 | CG | TYR A 420 | 35.063 | 68.583 | 57.856 | 1.00 | 10.31 | 6 | 3386 | CD | ARG A 424 | 25.862 | 64.465 | 55.212 | 1.00 | 11.09 | 6 |
| 3345 | CD1 | TYR A 420 | 34.258 | 69.238 | 58.754 | 1.00 | 13.30 | 6 | 3387 | NE | ARG A 424 | 24.666 | 64.721 | 54.412 | 1.00 | 10.91 | 7 |
| 3346 | CD2 | TYR A 420 | 34.669 | 68.523 | 56.512 | 1.00 | 13.25 | 6 | 3388 | CZ | ARG A 424 | 24.420 | 64.168 | 53.207 | 1.00 | 11.39 | 6 |
| 3347 | CE1 | TYR A 420 | 33.045 | 69.865 | 58.379 | 1.00 | 11.70 | 6 | 3389 | NH1 | ARG A 424 | 25.240 | 63.308 | 52.620 | 1.00 | 10.62 | 7 |
| 3348 | CE2 | TYR A 420 | 33.476 | 69.131 | 56.115 | 1.00 | 14.40 | 6 | 3390 | NH2 | ARG A 424 | 23.239 | 64.512 | 52.596 | 1.00 | 10.78 | 7 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3391 | N | LVS A 425 | 22.068 | 63.623 | 58.542 | 1.00 | 11.90 | 7 | 3433 | O | ASP A 429 | 20.026 | 60.024 | 59.967 | 1.00 | 13.16 | 8 |
| 3392 | CA | LVS A 425 | 20.937 | 63.080 | 59.290 | 1.00 | 11.75 | 6 | 3434 | CB | ASP A 429 | 18.927 | 57.501 | 58.471 | 1.00 | 12.81 | 6 |
| 3393 | C | LVS A 425 | 19.685 | 63.233 | 58.443 | 1.00 | 15.39 | 6 | 3435 | CG | ASP A 429 | 17.766 | 56.561 | 58.255 | 1.00 | 28.25 | 6 |
| 3394 | O | LVS A 425 | 19.444 | 64.340 | 58.036 | 1.00 | 14.23 | 8 | 3436 | OD1 | ASP A 429 | 17.727 | 55.530 | 58.940 | 1.00 | 20.84 | 8 |
| 3395 | CB | LVS A 425 | 20.801 | 63.854 | 60.626 | 1.00 | 13.68 | 6 | 3437 | OD2 | ASP A 429 | 16.804 | 56.870 | 57.490 | 1.00 | 27.47 | 8 |
| 3396 | CG | LVS A 425 | 19.617 | 63.271 | 61.494 | 1.00 | 14.44 | 6 | 3438 | N | VAL A 430 | 21.384 | 58.297 | 60.600 | 1.00 | 12.85 | 7 |
| 3397 | CD | LVS A 425 | 19.721 | 63.992 | 62.863 | 1.00 | 19.53 | 6 | 3439 | CA | VAL A 430 | 22.502 | 59.192 | 60.876 | 1.00 | 11.51 | 6 |
| 3398 | CE | LVS A 425 | 18.739 | 63.342 | 63.856 | 1.00 | 20.97 | 6 | 3440 | C | VAL A 430 | 23.816 | 58.621 | 60.371 | 1.00 | 13.31 | 6 |
| 3399 | NZ | LVS A 425 | 17.322 | 63.663 | 63.509 | 1.00 | 23.72 | 7 | 3441 | O | VAL A 430 | 23.993 | 57.405 | 60.522 | 1.00 | 12.49 | 8 |
| 3400 | N | PHE A 426 | 18.908 | 62.144 | 58.357 | 1.00 | 12.33 | 7 | 3442 | CB | VAL A 430 | 22.632 | 59.315 | 62.427 | 1.00 | 14.21 | 6 |
| 3401 | CA | PHE A 426 | 17.583 | 62.238 | 57.709 | 1.00 | 12.03 | 6 | 3443 | CG1 | VAL A 430 | 23.828 | 60.233 | 62.734 | 1.00 | 14.56 | 6 |
| 3402 | C | PHE A 426 | 16.651 | 61.481 | 58.706 | 1.00 | 11.05 | 6 | 3444 | CG2 | VAL A 430 | 21.373 | 59.955 | 63.033 | 1.00 | 14.79 | 6 |
| 3403 | O | PHE A 426 | 16.657 | 60.252 | 58.693 | 1.00 | 13.03 | 8 | 3445 | N | VAL A 431 | 24.721 | 59.432 | 59.826 | 1.00 | 12.54 | 7 |
| 3404 | CB | PHE A 426 | 17.608 | 61.450 | 56.397 | 1.00 | 13.23 | 6 | 3446 | CA | VAL A 431 | 26.043 | 58.933 | 59.434 | 1.00 | 11.58 | 6 |
| 3405 | CG | PHE A 426 | 16.260 | 61.449 | 55.699 | 1.00 | 12.58 | 6 | 3447 | C | VAL A 431 | 27.051 | 59.978 | 59.912 | 1.00 | 11.43 | 6 |
| 3406 | CD1 | PHE A 426 | 15.838 | 62.659 | 55.147 | 1.00 | 14.04 | 6 | 3448 | O | VAL A 431 | 26.847 | 61.129 | 59.603 | 1.00 | 12.12 | 8 |
| 3407 | CD2 | PHE A 426 | 15.515 | 60.300 | 55.571 | 1.00 | 14.55 | 6 | 3449 | CB | VAL A 431 | 26.250 | 58.685 | 57.905 | 1.00 | 12.54 | 6 |
| 3408 | CE1 | PHE A 426 | 14.594 | 62.715 | 54.490 | 1.00 | 13.58 | 6 | 3450 | CG1 | VAL A 431 | 27.698 | 58.199 | 57.615 | 1.00 | 10.81 | 6 |
| 3409 | CE2 | PHE A 426 | 14.264 | 60.345 | 54.906 | 1.00 | 15.67 | 6 | 3451 | CG2 | VAL A 431 | 25.254 | 57.657 | 57.400 | 1.00 | 13.14 | 6 |
| 3410 | CZ | PHE A 427 | 13.839 | 61.552 | 54.398 | 1.00 | 15.62 | 6 | 3452 | N | LEU A 432 | 27.976 | 59.557 | 60.800 | 1.00 | 10.48 | 7 |
| 3411 | N | PHE A 427 | 15.916 | 62.357 | 59.408 | 1.00 | 14.34 | 7 | 3453 | CA | LEU A 432 | 29.015 | 60.512 | 61.285 | 1.00 | 11.27 | 6 |
| 3412 | CA | PHE A 427 | 15.024 | 61.773 | 60.490 | 1.00 | 16.20 | 6 | 3454 | C | LEU A 432 | 30.317 | 60.140 | 60.583 | 1.00 | 11.12 | 6 |
| 3413 | C | PHE A 427 | 15.781 | 60.836 | 61.400 | 1.00 | 17.32 | 6 | 3455 | O | LEU A 432 | 30.708 | 58.961 | 60.577 | 1.00 | 11.86 | 6 |
| 3414 | O | PHE A 427 | 16.737 | 61.354 | 62.070 | 1.00 | 19.10 | 8 | 3456 | CB | LEU A 432 | 29.087 | 60.224 | 62.831 | 1.00 | 11.74 | 6 |
| 3415 | CB | PHE A 427 | 13.772 | 61.132 | 59.840 | 1.00 | 18.52 | 6 | 3457 | CG | LEU A 432 | 30.033 | 61.205 | 63.562 | 1.00 | 11.74 | 6 |
| 3416 | CG | PHE A 427 | 12.888 | 62.175 | 59.193 | 1.00 | 17.73 | 6 | 3458 | CD1 | LEU A 432 | 29.574 | 62.643 | 63.510 | 1.00 | 11.18 | 6 |
| 3417 | CD1 | PHE A 427 | 11.972 | 62.918 | 59.905 | 1.00 | 21.55 | 6 | 3459 | CD2 | LEU A 432 | 30.119 | 60.744 | 65.044 | 1.00 | 14.23 | 6 |
| 3418 | CD2 | PHE A 427 | 13.018 | 62.396 | 57.830 | 1.00 | 14.51 | 6 | 3460 | N | VAL A 433 | 30.987 | 61.141 | 59.978 | 1.00 | 11.73 | 7 |
| 3419 | CE1 | PHE A 427 | 11.188 | 63.858 | 59.276 | 1.00 | 18.85 | 6 | 3461 | CA | VAL A 433 | 32.162 | 60.867 | 59.131 | 1.00 | 9.07 | 6 |
| 3420 | CE2 | PHE A 427 | 12.246 | 63.336 | 57.185 | 1.00 | 16.68 | 6 | 3462 | C | VAL A 433 | 33.328 | 61.667 | 59.702 | 1.00 | 9.49 | 6 |
| 3421 | CZ | PHE A 427 | 11.311 | 64.087 | 57.906 | 1.00 | 19.85 | 6 | 3463 | O | VAL A 433 | 33.158 | 62.864 | 59.844 | 1.00 | 10.58 | 8 |
| 3422 | N | ASN A 428 | 15.546 | 59.522 | 61.442 | 1.00 | 15.71 | 7 | 3464 | CB | VAL A 433 | 31.899 | 61.334 | 57.674 | 1.00 | 10.62 | 6 |
| 3423 | CA | ASN A 428 | 16.284 | 58.735 | 62.433 | 1.00 | 17.74 | 6 | 3465 | CG1 | VAL A 433 | 33.173 | 61.088 | 56.812 | 1.00 | 11.05 | 6 |
| 3424 | C | ASN A 428 | 17.573 | 58.173 | 61.837 | 1.00 | 18.72 | 6 | 3466 | CG2 | VAL A 433 | 30.693 | 60.564 | 57.072 | 1.00 | 11.15 | 6 |
| 3425 | O | ASN A 428 | 18.307 | 57.587 | 62.639 | 1.00 | 17.57 | 8 | 3467 | N | ALA A 434 | 34.455 | 61.000 | 60.017 | 1.00 | 10.65 | 7 |
| 3426 | CB | ASN A 428 | 15.484 | 57.591 | 63.008 | 1.00 | 22.35 | 6 | 3468 | CA | ALA A 434 | 35.643 | 61.757 | 60.409 | 1.00 | 10.07 | 6 |
| 3427 | CG | ASN A 428 | 14.267 | 58.214 | 63.733 | 1.00 | 36.36 | 6 | 3469 | C | ALA A 434 | 36.742 | 61.603 | 59.363 | 1.00 | 11.73 | 6 |
| 3428 | OD1 | ASN A 428 | 14.452 | 59.092 | 64.570 | 1.00 | 38.45 | 8 | 3470 | O | ALA A 434 | 37.030 | 60.489 | 58.924 | 1.00 | 11.96 | 8 |
| 3429 | ND2 | ASN A 428 | 13.103 | 57.735 | 63.325 | 1.00 | 44.64 | 7 | 3471 | CB | ALA A 434 | 36.199 | 61.171 | 61.742 | 1.00 | 10.24 | 6 |
| 3430 | N | ASP A 429 | 17.867 | 58.370 | 60.547 | 1.00 | 15.06 | 7 | 3472 | N | ILE A 435 | 37.345 | 62.744 | 58.992 | 1.00 | 10.23 | 7 |
| 3431 | CA | ASP A 429 | 19.091 | 57.810 | 59.986 | 1.00 | 14.19 | 6 | 3473 | CA | ILE A 435 | 38.438 | 62.741 | 58.008 | 1.00 | 8.82 | 6 |
| 3432 | C | ASP A 429 | 20.222 | 58.816 | 60.103 | 1.00 | 11.55 | 6 | 3474 | C | ILE A 435 | 39.571 | 63.587 | 58.558 | 1.00 | 10.58 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3475 | O | ILE A 435 | 39.366 | 64.734 | 58.922 | 1.00 | 10.88 | 8 | 3517 | O | GLN A 440 | 52.198 | 62.543 | 61.812 | 1.00 | 18.55 | 8 |
| 3476 | CB | ILE A 435 | 37.961 | 63.408 | 56.674 | 1.00 | 10.84 | 6 | 3518 | CB | GLN A 440 | 52.905 | 63.422 | 59.081 | 1.00 | 23.60 | 6 |
| 3477 | CG1 | ILE A 435 | 36.749 | 62.608 | 56.120 | 1.00 | 11.49 | 6 | 3519 | CG | GLN A 440 | 53.543 | 62.971 | 57.761 | 1.00 | 37.17 | 6 |
| 3478 | CG2 | ILE A 435 | 39.146 | 63.352 | 55.689 | 1.00 | 10.37 | 6 | 3520 | CD | GLN A 440 | 54.248 | 61.634 | 57.810 | 1.00 | 48.48 | 6 |
| 3479 | CD1 | ILE A 435 | 36.230 | 63.228 | 54.758 | 1.00 | 13.59 | 6 | 3521 | OE1 | GLN A 440 | 55.292 | 61.462 | 58.444 | 1.00 | 57.64 | 8 |
| 3480 | N | ASN A 436 | 40.741 | 62.933 | 58.596 | 1.00 | 10.83 | 7 | 3522 | NE2 | GLN A 440 | 53.729 | 60.605 | 57.127 | 1.00 | 54.59 | 7 |
| 3481 | CA | ASN A 436 | 41.963 | 63.646 | 58.943 | 1.00 | 11.64 | 6 | 3523 | N | SER A 441 | 50.115 | 63.161 | 61.192 | 1.00 | 13.09 | 7 |
| 3482 | C | ASN A 436 | 42.852 | 63.653 | 57.715 | 1.00 | 9.83 | 6 | 3524 | CA | SER A 441 | 49.738 | 63.516 | 62.559 | 1.00 | 13.14 | 6 |
| 3483 | O | ASN A 436 | 43.367 | 62.621 | 57.309 | 1.00 | 12.85 | 8 | 3525 | C | SER A 441 | 48.481 | 62.739 | 62.958 | 1.00 | 18.60 | 6 |
| 3484 | CB | ASN A 436 | 42.711 | 62.821 | 60.036 | 1.00 | 12.59 | 6 | 3526 | O | SER A 441 | 47.524 | 62.718 | 62.168 | 1.00 | 15.27 | 8 |
| 3485 | CG | ASN A 436 | 44.030 | 63.480 | 60.383 | 1.00 | 12.87 | 6 | 3527 | CB | SER A 441 | 49.451 | 65.025 | 62.702 | 1.00 | 16.00 | 6 |
| 3486 | OD1 | ASN A 436 | 44.422 | 64.602 | 60.026 | 1.00 | 13.07 | 8 | 3528 | OG | SER A 441 | 50.658 | 65.770 | 62.516 | 1.00 | 17.34 | 8 |
| 3487 | ND2 | ASN A 436 | 44.789 | 62.721 | 61.224 | 1.00 | 13.56 | 7 | 3529 | N | SER A 442 | 48.417 | 62.251 | 64.198 | 1.00 | 13.46 | 7 |
| 3488 | N | ARG A 437 | 43.055 | 64.891 | 57.181 | 1.00 | 10.03 | 7 | 3530 | CA | SER A 442 | 47.177 | 61.703 | 64.730 | 1.00 | 13.64 | 6 |
| 3489 | CA | ARG A 437 | 43.878 | 64.887 | 55.958 | 1.00 | 9.39 | 6 | 3531 | C | SER A 442 | 46.581 | 62.835 | 65.599 | 1.00 | 14.33 | 6 |
| 3490 | C | ARG A 437 | 45.362 | 64.725 | 56.267 | 1.00 | 10.71 | 6 | 3532 | O | SER A 442 | 47.366 | 63.761 | 65.974 | 1.00 | 15.22 | 8 |
| 3491 | O | ARG A 437 | 46.117 | 64.552 | 55.310 | 1.00 | 12.32 | 8 | 3533 | CB | SER A 442 | 47.452 | 60.598 | 65.791 | 1.00 | 15.48 | 6 |
| 3492 | CB | ARG A 437 | 43.673 | 66.201 | 55.161 | 1.00 | 13.58 | 6 | 3534 | OG | SER A 442 | 48.033 | 59.420 | 65.203 | 1.00 | 19.49 | 8 |
| 3493 | CG | ARG A 437 | 44.296 | 67.415 | 55.869 | 1.00 | 12.80 | 6 | 3535 | N | TYR A 443 | 45.302 | 62.845 | 65.817 | 1.00 | 13.24 | 7 |
| 3494 | CD | ARG A 437 | 44.031 | 68.719 | 55.043 | 1.00 | 11.13 | 6 | 3536 | CA | TYR A 443 | 44.693 | 63.886 | 66.694 | 1.00 | 12.26 | 6 |
| 3495 | NE | ARG A 437 | 44.772 | 69.847 | 55.738 | 1.00 | 10.90 | 7 | 3537 | C | TYR A 443 | 43.877 | 63.156 | 67.749 | 1.00 | 14.89 | 6 |
| 3496 | CZ | ARG A 437 | 44.957 | 71.046 | 55.195 | 1.00 | 14.88 | 6 | 3538 | O | TYR A 443 | 43.032 | 62.293 | 67.451 | 1.00 | 14.44 | 8 |
| 3497 | NH1 | ARG A 437 | 44.521 | 71.299 | 53.948 | 1.00 | 11.67 | 7 | 3539 | CB | TYR A 443 | 43.772 | 64.824 | 65.860 | 1.00 | 13.59 | 6 |
| 3498 | NH2 | ARG A 437 | 45.406 | 72.058 | 55.947 | 1.00 | 13.84 | 7 | 3540 | CG | TYR A 443 | 44.592 | 65.807 | 65.009 | 1.00 | 10.92 | 6 |
| 3499 | N | ASN A 438 | 45.779 | 65.035 | 57.513 | 1.00 | 11.11 | 7 | 3541 | CD1 | TYR A 443 | 45.124 | 66.940 | 65.629 | 1.00 | 12.95 | 6 |
| 3500 | CA | ASN A 438 | 47.255 | 65.048 | 57.734 | 1.00 | 12.20 | 6 | 3542 | CD2 | TYR A 443 | 44.836 | 65.549 | 63.667 | 1.00 | 11.89 | 6 |
| 3501 | C | ASN A 438 | 47.780 | 63.623 | 57.869 | 1.00 | 13.73 | 6 | 3543 | CE1 | TYR A 443 | 45.908 | 67.843 | 64.882 | 1.00 | 11.89 | 6 |
| 3502 | O | ASN A 438 | 47.440 | 62.900 | 58.830 | 1.00 | 12.56 | 8 | 3544 | CE2 | TYR A 443 | 45.595 | 66.474 | 62.914 | 1.00 | 11.54 | 6 |
| 3503 | CB | ASN A 438 | 47.474 | 65.787 | 59.071 | 1.00 | 13.49 | 6 | 3545 | CZ | TYR A 443 | 46.107 | 67.595 | 63.551 | 1.00 | 12.16 | 6 |
| 3504 | CG | ASN A 438 | 48.921 | 66.167 | 59.255 | 1.00 | 13.92 | 6 | 3546 | OH | TYR A 443 | 46.871 | 68.508 | 62.811 | 1.00 | 15.42 | 8 |
| 3505 | OD1 | ASN A 438 | 49.775 | 65.335 | 58.985 | 1.00 | 15.45 | 8 | 3547 | N | SER A 444 | 43.976 | 63.663 | 69.008 | 1.00 | 14.60 | 7 |
| 3506 | ND2 | ASN A 438 | 49.263 | 67.376 | 59.700 | 1.00 | 13.51 | 7 | 3548 | CA | SER A 444 | 43.034 | 63.232 | 70.040 | 1.00 | 14.67 | 6 |
| 3507 | N | THR A 439 | 48.650 | 63.224 | 56.949 | 1.00 | 11.49 | 7 | 3549 | C | SER A 444 | 41.698 | 64.002 | 69.912 | 1.00 | 13.95 | 6 |
| 3508 | CA | THR A 439 | 49.087 | 61.822 | 56.883 | 1.00 | 12.77 | 6 | 3550 | O | SER A 444 | 41.739 | 65.229 | 69.879 | 1.00 | 16.35 | 8 |
| 3509 | C | THR A 439 | 50.271 | 61.585 | 57.846 | 1.00 | 14.69 | 6 | 3551 | CB | SER A 444 | 43.620 | 63.684 | 71.418 | 1.00 | 17.27 | 6 |
| 3510 | O | THR A 439 | 50.750 | 60.450 | 57.917 | 1.00 | 16.23 | 8 | 3552 | OG | SER A 444 | 44.701 | 62.764 | 71.733 | 1.00 | 18.88 | 8 |
| 3511 | CB | THR A 439 | 49.518 | 61.431 | 55.456 | 1.00 | 16.48 | 6 | 3553 | N | ILE A 445 | 40.628 | 63.265 | 69.758 | 1.00 | 15.00 | 7 |
| 3512 | OG1 | THR A 439 | 50.542 | 62.330 | 54.990 | 1.00 | 17.73 | 8 | 3554 | CA | ILE A 445 | 39.303 | 63.892 | 69.559 | 1.00 | 13.10 | 6 |
| 3513 | CG2 | THR A 439 | 48.284 | 61.611 | 54.554 | 1.00 | 15.47 | 6 | 3555 | C | ILE A 445 | 38.498 | 63.757 | 70.863 | 1.00 | 14.11 | 6 |
| 3514 | N | GLN A 440 | 50.666 | 62.669 | 58.501 | 1.00 | 14.00 | 7 | 3556 | O | ILE A 445 | 37.935 | 62.703 | 71.131 | 1.00 | 17.51 | 8 |
| 3515 | CA | GLN A 440 | 51.778 | 62.467 | 59.481 | 1.00 | 16.61 | 6 | 3557 | CB | ILE A 445 | 38.537 | 63.188 | 68.403 | 1.00 | 14.59 | 6 |
| 3516 | C | GLN A 440 | 51.339 | 62.729 | 60.910 | 1.00 | 19.80 | 6 | 3558 | CG1 | ILE A 445 | 39.386 | 63.120 | 67.136 | 1.00 | 15.39 | 6 |

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|------|---------------|--------|--------|--------|------------|---|------|---------------|--------|--------|--------|------------|---|
| 3559 | CG2 ILE A 445 | 37.159 | 63.906 | 68.223 | 1.00 16.44 | 6 | 3596 | CA ALA A 451 | 22.898 | 62.330 | 66.941 | 1.00 16.96 | 6 |
| 3560 | CD1 ILE A 445 | 39.772 | 64.500 | 66.533 | 1.00 15.53 | 6 | 3597 | C ALA A 451 | 22.799 | 60.830 | 66.879 | 1.00 15.04 | 6 |
| 3561 | N SER A 446 | 38.309 | 64.925 | 71.501 | 1.00 15.73 | 7 | 3598 | O ALA A 451 | 21.681 | 60.282 | 66.900 | 1.00 15.44 | 8 |
| 3562 | CA SER A 446 | 37.450 | 65.018 | 72.680 | 1.00 16.64 | 6 | 3599 | CB ALA A 451 | 22.212 | 62.946 | 65.681 | 1.00 16.26 | 6 |
| 3563 | C SER A 446 | 36.394 | 66.091 | 72.415 | 1.00 18.39 | 6 | 3600 | N LEU A 452 | 23.929 | 60.083 | 66.788 | 1.00 14.57 | 7 |
| 3564 | O SER A 446 | 36.592 | 67.021 | 71.653 | 1.00 18.43 | 8 | 3601 | CA LEU A 452 | 23.803 | 58.623 | 66.814 | 1.00 12.45 | 6 |
| 3565 | CB SER A 446 | 38.248 | 65.398 | 73.972 | 1.00 18.77 | 6 | 3602 | C LEU A 452 | 23.170 | 58.200 | 68.158 | 1.00 17.32 | 6 |
| 3566 | OG SER A 446 | 38.784 | 66.689 | 73.750 | 1.00 24.38 | 8 | 3603 | O LEU A 452 | 23.505 | 58.727 | 69.218 | 1.00 17.00 | 8 |
| 3567 | N GLY A 447 | 35.263 | 65.958 | 73.091 | 1.00 19.05 | 7 | 3604 | CB LEU A 452 | 25.201 | 57.989 | 66.779 | 1.00 14.27 | 6 |
| 3568 | CA GLY A 447 | 34.169 | 66.916 | 73.050 | 1.00 17.05 | 6 | 3605 | CG LEU A 452 | 25.854 | 58.082 | 65.380 | 1.00 14.43 | 6 |
| 3569 | C GLY A 447 | 33.253 | 66.660 | 71.829 | 1.00 20.26 | 6 | 3606 | CD1 LEU A 452 | 27.344 | 57.716 | 65.610 | 1.00 13.81 | 6 |
| 3570 | O GLY A 447 | 32.491 | 67.554 | 71.467 | 1.00 19.38 | 8 | 3607 | CD2 LEU A 452 | 25.263 | 57.102 | 64.375 | 1.00 14.40 | 6 |
| 3571 | N LEU A 448 | 33.487 | 65.502 | 71.171 | 1.00 13.94 | 7 | 3608 | N PRO A 453 | 22.383 | 57.163 | 68.080 | 1.00 16.12 | 7 |
| 3572 | CA LEU A 448 | 32.625 | 65.262 | 69.967 | 1.00 15.40 | 6 | 3609 | CA PRO A 453 | 21.808 | 56.539 | 69.305 | 1.00 18.87 | 6 |
| 3573 | C LEU A 448 | 31.245 | 64.853 | 70.386 | 1.00 16.78 | 6 | 3610 | C PRO A 453 | 22.936 | 55.882 | 70.090 | 1.00 19.68 | 6 |
| 3574 | O LEU A 448 | 31.018 | 63.906 | 71.155 | 1.00 17.47 | 8 | 3611 | O PRO A 453 | 24.039 | 55.532 | 69.686 | 1.00 18.19 | 8 |
| 3575 | CB LEU A 448 | 33.312 | 64.155 | 69.144 | 1.00 14.08 | 6 | 3612 | CB PRO A 453 | 20.796 | 55.523 | 68.880 | 1.00 20.41 | 6 |
| 3576 | CG LEU A 448 | 32.578 | 63.628 | 67.903 | 1.00 15.34 | 6 | 3613 | CG PRO A 453 | 20.615 | 55.743 | 67.392 | 1.00 21.35 | 6 |
| 3577 | CD1 LEU A 448 | 32.403 | 64.740 | 66.845 | 1.00 16.18 | 6 | 3614 | CD PRO A 453 | 21.806 | 56.582 | 66.872 | 1.00 16.78 | 6 |
| 3578 | CD2 LEU A 448 | 33.283 | 62.449 | 67.256 | 1.00 13.42 | 6 | 3615 | N ASN A 454 | 22.619 | 55.684 | 71.406 | 1.00 14.58 | 7 |
| 3579 | N GLN A 449 | 30.221 | 65.509 | 69.814 | 1.00 13.16 | 7 | 3616 | CA ASN A 454 | 23.630 | 55.025 | 72.244 | 1.00 14.89 | 6 |
| 3580 | CA GLN A 449 | 28.812 | 65.224 | 70.018 | 1.00 14.91 | 6 | 3617 | C ASN A 454 | 24.085 | 53.704 | 71.712 | 1.00 18.47 | 6 |
| 3581 | C GLN A 449 | 28.209 | 64.630 | 68.734 | 1.00 16.76 | 6 | 3618 | O ASN A 454 | 23.320 | 52.881 | 71.168 | 1.00 17.84 | 8 |
| 3582 | O GLN A 449 | 28.754 | 64.827 | 67.645 | 1.00 13.94 | 8 | 3619 | CB ASN A 454 | 22.851 | 54.705 | 73.573 | 1.00 17.80 | 6 |
| 3583 | CB AGLN A 449 | 28.054 | 66.486 | 70.470 | 0.50 18.23 | 6 | 3620 | CG ASN A 454 | 22.656 | 55.933 | 74.421 | 1.00 24.08 | 6 |
| 3584 | CG AGLN A 449 | 28.884 | 67.206 | 71.540 | 0.50 24.01 | 6 | 3621 | OD1 ASN A 454 | 23.071 | 57.055 | 74.201 | 1.00 19.24 | 8 |
| 3585 | CD AGLN A 449 | 28.211 | 68.188 | 72.449 | 0.50 23.44 | 6 | 3622 | ND2 ASN A 454 | 21.941 | 55.757 | 75.554 | 1.00 24.42 | 7 |
| 3586 | OE1AGLN A 449 | 28.812 | 68.606 | 73.455 | 0.50 32.55 | 8 | 3623 | N GLY A 455 | 25.378 | 53.451 | 71.950 | 1.00 17.75 | 7 |
| 3587 | NE2AGLN A 449 | 26.984 | 68.573 | 72.134 | 0.50 32.22 | 7 | 3624 | CA GLY A 455 | 25.919 | 52.156 | 71.553 | 1.00 20.13 | 6 |
| 3588 | CB BGLN A 449 | 27.974 | 66.473 | 70.339 | 0.50 13.26 | 6 | 3625 | C GLY A 455 | 27.422 | 52.289 | 71.172 | 1.00 17.39 | 6 |
| 3589 | CG BGLN A 449 | 28.536 | 67.122 | 71.620 | 0.50 17.72 | 6 | 3626 | O GLY A 455 | 27.899 | 53.393 | 71.080 | 1.00 19.07 | 8 |
| 3590 | CD BGLN A 449 | 28.037 | 66.396 | 72.844 | 0.50 16.00 | 6 | 3627 | N SER A 456 | 27.916 | 51.112 | 70.814 | 1.00 18.37 | 7 |
| 3591 | OE1BGLN A 449 | 28.776 | 65.702 | 73.511 | 0.50 22.43 | 8 | 3628 | CA SER A 456 | 29.286 | 51.073 | 70.261 | 1.00 17.34 | 6 |
| 3592 | NE2BGLN A 449 | 26.759 | 66.550 | 73.145 | 0.50 23.34 | 7 | 3629 | C SER A 456 | 29.173 | 50.927 | 68.725 | 1.00 17.80 | 6 |
| 3593 | N THR A 450 | 27.085 | 63.965 | 68.897 | 1.00 15.61 | 7 | 3630 | O SER A 456 | 28.322 | 50.199 | 68.220 | 1.00 20.53 | 8 |
| 3594 | CA THR A 450 | 26.481 | 63.264 | 67.761 | 1.00 13.97 | 6 | 3631 | CB SER A 456 | 29.916 | 49.747 | 70.778 | 1.00 22.39 | 6 |
| 3595 | C THR A 450 | 24.998 | 63.001 | 67.994 | 1.00 16.43 | 6 | 3632 | OG SER A 456 | 30.178 | 49.998 | 72.161 | 1.00 30.42 | 8 |
| 3596 | O THR A 450 | 24.528 | 62.925 | 69.160 | 1.00 16.61 | 8 | 3633 | N TYR A 457 | 30.024 | 51.683 | 68.013 | 1.00 15.08 | 7 |
| 3597 | CB THR A 450 | 27.216 | 61.912 | 67.566 | 1.00 15.00 | 6 | 3634 | CA TYR A 457 | 29.941 | 51.627 | 66.559 | 1.00 13.18 | 6 |
| 3598 | OG1 THR A 450 | 26.686 | 61.176 | 66.471 | 1.00 15.07 | 8 | 3635 | C TYR A 457 | 31.301 | 51.229 | 65.961 | 1.00 14.20 | 6 |
| 3599 | CG2 THR A 450 | 27.007 | 61.016 | 68.814 | 1.00 18.27 | 6 | 3636 | O TYR A 457 | 32.257 | 51.915 | 66.259 | 1.00 16.66 | 8 |
| 3595 | N ALA A 451 | 24.286 | 62.806 | 66.886 | 1.00 15.10 | 7 | 3637 | CB TYR A 457 | 29.564 | 53.017 | 65.941 | 1.00 17.47 | 6 |

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|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 3638 | CG | TYR | A | 457 | 28.122 | 53.387 | 66.241 | 1.00 | 15.26 | 6 | 3680 | C | SER | A | 462 | 38.011 | 48.422 | 58.907 | 1.00 | 17.10 | 6 |
| 3639 | CD1 | TYR | A | 457 | 27.799 | 53.933 | 67.497 | 1.00 | 15.37 | 6 | 3681 | O | SER | A | 462 | 38.878 | 47.546 | 58.763 | 1.00 | 16.40 | 8 |
| 3640 | CD2 | TYR | A | 457 | 27.077 | 53.174 | 65.325 | 1.00 | 16.16 | 6 | 3682 | CB | SER | A | 462 | 36.316 | 46.813 | 57.987 | 1.00 | 19.17 | 6 |
| 3641 | CE1 | TYR | A | 457 | 26.521 | 54.297 | 67.873 | 1.00 | 15.82 | 6 | 3683 | OG | SER | A | 462 | 34.914 | 46.479 | 57.974 | 1.00 | 20.76 | 8 |
| 3642 | CE2 | TYR | A | 457 | 25.768 | 53.516 | 65.671 | 1.00 | 15.99 | 6 | 3684 | N | GLY | A | 463 | 38.369 | 49.689 | 59.115 | 1.00 | 13.98 | 7 |
| 3643 | CZ | TYR | A | 457 | 25.523 | 54.070 | 66.928 | 1.00 | 16.37 | 6 | 3685 | CA | GLY | A | 463 | 39.781 | 50.089 | 59.271 | 1.00 | 14.97 | 6 |
| 3644 | OH | TYR | A | 457 | 24.210 | 54.401 | 67.218 | 1.00 | 16.11 | 8 | 3686 | C | GLY | A | 463 | 40.533 | 50.140 | 57.949 | 1.00 | 15.42 | 6 |
| 3645 | N | ALA | A | 458 | 31.329 | 50.211 | 65.128 | 1.00 | 14.59 | 7 | 3687 | O | GLY | A | 463 | 41.745 | 50.387 | 57.984 | 1.00 | 15.84 | 8 |
| 3646 | CA | ALA | A | 458 | 32.601 | 49.943 | 64.445 | 1.00 | 17.03 | 6 | 3688 | N | LEU | A | 464 | 39.816 | 50.043 | 56.808 | 1.00 | 12.86 | 7 |
| 3647 | C | ALA | A | 458 | 32.686 | 50.915 | 63.247 | 1.00 | 14.66 | 6 | 3689 | CA | LEU | A | 464 | 40.559 | 50.113 | 55.525 | 1.00 | 10.93 | 6 |
| 3648 | O | ALA | A | 458 | 31.654 | 51.326 | 62.731 | 1.00 | 14.84 | 8 | 3690 | C | LEU | A | 464 | 41.370 | 51.420 | 55.427 | 1.00 | 12.62 | 6 |
| 3649 | CB | ALA | A | 458 | 32.638 | 48.538 | 63.857 | 1.00 | 17.50 | 6 | 3691 | O | LEU | A | 464 | 42.484 | 51.408 | 54.854 | 1.00 | 14.36 | 8 |
| 3650 | N | ASP | A | 459 | 33.942 | 51.128 | 62.831 | 1.00 | 13.42 | 7 | 3692 | CB | LEU | A | 464 | 39.487 | 50.148 | 54.402 | 1.00 | 13.24 | 6 |
| 3651 | CA | ASP | A | 459 | 34.082 | 51.858 | 61.521 | 1.00 | 11.91 | 6 | 3693 | CG | LEU | A | 464 | 40.083 | 50.223 | 52.969 | 1.00 | 14.42 | 6 |
| 3652 | C | ASP | A | 459 | 33.472 | 51.048 | 60.410 | 1.00 | 12.75 | 6 | 3694 | CD1 | LEU | A | 464 | 40.800 | 48.892 | 52.620 | 1.00 | 15.93 | 6 |
| 3653 | O | ASP | A | 459 | 33.679 | 49.834 | 60.222 | 1.00 | 13.42 | 8 | 3695 | CD2 | LEU | A | 464 | 38.971 | 50.469 | 51.967 | 1.00 | 14.00 | 6 |
| 3654 | CB | ASP | A | 459 | 35.567 | 52.007 | 61.258 | 1.00 | 12.66 | 6 | 3696 | N | LEU | A | 465 | 40.797 | 52.526 | 55.872 | 1.00 | 11.79 | 7 |
| 3655 | CG | ASP | A | 459 | 35.984 | 52.522 | 59.876 | 1.00 | 13.56 | 6 | 3697 | CA | LEU | A | 465 | 41.473 | 53.824 | 55.761 | 1.00 | 12.51 | 6 |
| 3656 | OD1 | ASP | A | 459 | 35.143 | 53.232 | 59.328 | 1.00 | 12.36 | 8 | 3698 | C | LEU | A | 465 | 41.953 | 54.319 | 57.114 | 1.00 | 13.32 | 6 |
| 3657 | OD2 | ASP | A | 459 | 37.109 | 52.170 | 59.441 | 1.00 | 14.11 | 8 | 3699 | O | LEU | A | 465 | 41.873 | 55.518 | 57.401 | 1.00 | 16.12 | 8 |
| 3658 | N | TYR | A | 460 | 32.581 | 51.730 | 59.662 | 1.00 | 11.96 | 7 | 3700 | CB | LEU | A | 465 | 40.510 | 54.894 | 55.130 | 1.00 | 12.90 | 6 |
| 3659 | CA | TYR | A | 460 | 31.927 | 51.022 | 58.513 | 1.00 | 13.29 | 6 | 3701 | CG | LEU | A | 465 | 40.090 | 54.441 | 53.714 | 1.00 | 12.88 | 6 |
| 3660 | C | TYR | A | 460 | 32.905 | 50.541 | 57.467 | 1.00 | 16.04 | 6 | 3702 | CD1 | LEU | A | 465 | 39.162 | 55.509 | 53.111 | 1.00 | 14.96 | 6 |
| 3661 | O | TYR | A | 460 | 32.617 | 49.627 | 56.683 | 1.00 | 15.32 | 8 | 3703 | CD2 | LEU | A | 465 | 41.263 | 54.191 | 52.777 | 1.00 | 14.83 | 6 |
| 3662 | CB | TYR | A | 460 | 30.909 | 52.021 | 57.931 | 1.00 | 13.60 | 6 | 3704 | N | GLY | A | 466 | 42.237 | 53.348 | 58.043 | 1.00 | 14.06 | 7 |
| 3663 | CG | TYR | A | 460 | 29.970 | 51.418 | 56.899 | 1.00 | 13.06 | 6 | 3705 | CA | GLY | A | 466 | 42.789 | 53.800 | 59.336 | 1.00 | 14.74 | 6 |
| 3664 | CD1 | TYR | A | 460 | 28.809 | 50.815 | 57.400 | 1.00 | 11.63 | 6 | 3706 | C | GLY | A | 466 | 41.735 | 54.095 | 60.400 | 1.00 | 14.06 | 6 |
| 3665 | CD2 | TYR | A | 460 | 30.215 | 51.365 | 55.532 | 1.00 | 16.49 | 6 | 3707 | O | GLY | A | 466 | 42.061 | 54.643 | 61.479 | 1.00 | 15.13 | 8 |
| 3666 | CE1 | TYR | A | 460 | 27.838 | 50.274 | 56.514 | 1.00 | 15.86 | 6 | 3708 | N | GLY | A | 467 | 40.451 | 53.817 | 60.125 | 1.00 | 13.86 | 7 |
| 3667 | CE2 | TYR | A | 460 | 29.278 | 50.783 | 54.662 | 1.00 | 15.66 | 6 | 3709 | CA | GLY | A | 467 | 39.357 | 54.137 | 61.045 | 1.00 | 11.80 | 6 |
| 3668 | CZ | TYR | A | 460 | 28.098 | 50.257 | 55.165 | 1.00 | 17.45 | 6 | 3710 | C | GLY | A | 467 | 39.321 | 53.244 | 62.311 | 1.00 | 14.35 | 6 |
| 3669 | OH | TYR | A | 460 | 27.209 | 49.696 | 54.262 | 1.00 | 16.44 | 8 | 3711 | O | GLY | A | 467 | 40.083 | 52.261 | 62.394 | 1.00 | 16.59 | 8 |
| 3670 | N | LEU | A | 461 | 34.057 | 51.242 | 57.374 | 1.00 | 13.04 | 7 | 3712 | N | ASN | A | 468 | 38.509 | 53.696 | 63.236 | 1.00 | 15.29 | 7 |
| 3671 | CA | LEU | A | 461 | 35.137 | 50.814 | 56.424 | 1.00 | 13.89 | 6 | 3713 | CA | ASN | A | 468 | 38.483 | 53.050 | 64.569 | 1.00 | 14.61 | 6 |
| 3672 | C | LEU | A | 461 | 36.026 | 49.742 | 57.023 | 1.00 | 14.71 | 6 | 3714 | C | ASN | A | 468 | 37.007 | 52.960 | 64.963 | 1.00 | 15.14 | 6 |
| 3673 | O | LEU | A | 461 | 36.992 | 49.331 | 56.369 | 1.00 | 13.39 | 8 | 3715 | O | ASN | A | 468 | 36.145 | 53.679 | 64.418 | 1.00 | 15.07 | 8 |
| 3674 | CB | LEU | A | 461 | 35.968 | 52.115 | 55.171 | 1.00 | 13.08 | 6 | 3716 | CB | ASN | A | 468 | 39.253 | 54.012 | 65.515 | 1.00 | 16.45 | 6 |
| 3675 | CG | LEU | A | 461 | 35.299 | 53.075 | 55.149 | 1.00 | 13.44 | 6 | 3717 | CG | ASN | A | 468 | 38.730 | 55.429 | 65.538 | 1.00 | 17.15 | 6 |
| 3676 | CD1 | LEU | A | 461 | 35.968 | 54.453 | 55.284 | 1.00 | 14.44 | 6 | 3718 | OD1 | ASN | A | 468 | 39.013 | 56.375 | 64.739 | 1.00 | 19.92 | 8 |
| 3677 | CD2 | LEU | A | 461 | 35.485 | 52.526 | 53.743 | 1.00 | 16.37 | 6 | 3719 | ND2 | ASN | A | 468 | 37.812 | 55.710 | 66.490 | 1.00 | 16.39 | 7 |
| 3678 | N | SER | A | 462 | 35.746 | 49.218 | 58.222 | 1.00 | 15.11 | 7 | 3720 | N | GLY | A | 469 | 36.787 | 52.285 | 66.076 | 1.00 | 16.49 | 7 |
| 3679 | CA | SER | A | 462 | 36.521 | 48.122 | 58.810 | 1.00 | 16.17 | 6 | 3721 | CA | GLY | A | 469 | 35.415 | 52.189 | 66.624 | 1.00 | 16.85 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|------------|--------|--------|--------|------|-------|---|
| 3722 | C | GLY A 469 | 35.261 | 53.309 | 67.640 | 1.00 | 14.55 | 6 | 3764 | CA | SER A 476 | 28.563 | 62.222 | 73.451 | 1.00 | 14.26 | 6 |
| 3723 | O | GLY A 469 | 36.191 | 53.919 | 68.176 | 1.00 | 17.51 | 8 | 3765 | C | SER A 476 | 29.384 | 61.026 | 72.974 | 1.00 | 17.38 | 6 |
| 3724 | N | ILE A 470 | 33.976 | 53.624 | 67.954 | 1.00 | 14.83 | 7 | 3766 | O | SER A 476 | 29.103 | 59.902 | 73.358 | 1.00 | 18.38 | 8 |
| 3725 | CA | ILE A 470 | 33.623 | 54.650 | 68.921 | 1.00 | 14.09 | 6 | 3767 | CB | ASER A 476 | 28.931 | 62.557 | 74.900 | 0.70 | 19.66 | 6 |
| 3726 | C | ILE A 470 | 32.518 | 54.102 | 69.860 | 1.00 | 13.92 | 6 | 3768 | OG | ASER A 476 | 28.330 | 63.803 | 75.257 | 0.70 | 22.12 | 8 |
| 3727 | O | ILE A 470 | 31.867 | 53.108 | 69.553 | 1.00 | 19.57 | 8 | 3769 | CB | BSER A 476 | 28.870 | 62.465 | 74.932 | 0.30 | 18.16 | 6 |
| 3728 | CB | ILE A 470 | 33.155 | 56.004 | 68.368 | 1.00 | 16.37 | 6 | 3768 | OG | BSER A 476 | 30.220 | 62.822 | 75.127 | 0.30 | 20.85 | 8 |
| 3729 | CG1 | ILE A 470 | 31.948 | 55.753 | 67.429 | 1.00 | 17.51 | 6 | 3769 | N | VAL A 477 | 30.430 | 61.284 | 72.188 | 1.00 | 15.08 | 7 |
| 3730 | CG2 | ILE A 470 | 34.319 | 56.652 | 67.581 | 1.00 | 16.76 | 6 | 3770 | CA | VAL A 477 | 31.322 | 60.248 | 71.766 | 1.00 | 16.01 | 6 |
| 3731 | CD1 | ILE A 470 | 31.315 | 57.104 | 67.032 | 1.00 | 15.78 | 6 | 3771 | C | VAL A 477 | 32.549 | 60.211 | 72.699 | 1.00 | 14.42 | 6 |
| 3732 | N | SER A 471 | 32.408 | 54.804 | 70.980 | 1.00 | 15.71 | 7 | 3772 | O | VAL A 477 | 33.117 | 61.277 | 72.913 | 1.00 | 16.73 | 8 |
| 3733 | CA | SER A 471 | 31.268 | 54.477 | 71.903 | 1.00 | 14.51 | 6 | 3773 | CB | VAL A 477 | 31.852 | 60.539 | 70.320 | 1.00 | 12.17 | 6 |
| 3734 | C | SER A 471 | 30.497 | 55.755 | 72.165 | 1.00 | 14.83 | 6 | 3774 | CG1 | VAL A 477 | 32.718 | 59.377 | 69.872 | 1.00 | 15.08 | 6 |
| 3735 | O | SER A 471 | 31.107 | 56.814 | 72.402 | 1.00 | 17.55 | 8 | 3775 | CG2 | VAL A 477 | 30.665 | 60.682 | 69.389 | 1.00 | 13.12 | 6 |
| 3736 | CB | SER A 471 | 32.024 | 54.018 | 73.220 | 1.00 | 22.00 | 6 | 3776 | N | ALA A 478 | 32.802 | 59.035 | 73.236 | 1.00 | 17.39 | 7 |
| 3737 | OG | SER A 471 | 30.967 | 53.933 | 74.176 | 1.00 | 27.40 | 8 | 3777 | CA | ALA A 478 | 33.956 | 58.962 | 74.181 | 1.00 | 17.45 | 6 |
| 3738 | N | VAL A 472 | 29.172 | 55.712 | 72.054 | 1.00 | 14.69 | 7 | 3778 | C | ALA A 478 | 35.248 | 59.401 | 73.501 | 1.00 | 19.79 | 6 |
| 3739 | CA | VAL A 472 | 28.298 | 56.834 | 72.186 | 1.00 | 14.15 | 6 | 3779 | O | ALA A 478 | 35.398 | 59.204 | 72.298 | 1.00 | 15.95 | 8 |
| 3740 | C | VAL A 472 | 27.380 | 56.696 | 73.425 | 1.00 | 15.07 | 6 | 3780 | CB | ALA A 478 | 34.031 | 57.543 | 74.731 | 1.00 | 18.76 | 6 |
| 3741 | O | VAL A 472 | 26.764 | 55.638 | 73.563 | 1.00 | 19.05 | 8 | 3781 | N | SER A 479 | 36.152 | 60.069 | 74.181 | 1.00 | 15.72 | 7 |
| 3742 | CB | VAL A 472 | 27.433 | 56.903 | 70.900 | 1.00 | 14.81 | 6 | 3782 | CA | SER A 479 | 37.405 | 60.518 | 73.501 | 1.00 | 17.20 | 6 |
| 3743 | CG1 | VAL A 472 | 26.446 | 58.057 | 70.970 | 1.00 | 18.40 | 6 | 3783 | C | SER A 479 | 38.170 | 59.392 | 72.855 | 1.00 | 16.18 | 6 |
| 3744 | CG2 | VAL A 472 | 28.376 | 57.153 | 69.691 | 1.00 | 18.40 | 6 | 3784 | O | SER A 479 | 38.177 | 58.231 | 73.329 | 1.00 | 16.38 | 8 |
| 3745 | N | SER A 473 | 27.351 | 57.767 | 74.184 | 1.00 | 15.80 | 7 | 3785 | CB | SER A 479 | 38.262 | 61.218 | 74.569 | 1.00 | 23.12 | 6 |
| 3746 | CA | SER A 473 | 26.386 | 57.736 | 75.312 | 1.00 | 16.44 | 6 | 3786 | OG | SER A 479 | 37.554 | 62.348 | 75.047 | 1.00 | 22.40 | 8 |
| 3747 | C | SER A 473 | 25.711 | 59.073 | 75.420 | 1.00 | 16.40 | 6 | 3787 | N | PHE A 480 | 38.774 | 59.656 | 71.674 | 1.00 | 16.00 | 7 |
| 3748 | O | SER A 473 | 26.435 | 60.084 | 75.548 | 1.00 | 19.98 | 8 | 3788 | CA | PHE A 480 | 39.449 | 58.638 | 70.881 | 1.00 | 15.01 | 6 |
| 3749 | CB | SER A 473 | 27.214 | 57.446 | 76.594 | 1.00 | 21.00 | 6 | 3789 | C | PHE A 480 | 40.575 | 59.308 | 70.092 | 1.00 | 14.53 | 6 |
| 3750 | OG | SER A 473 | 26.284 | 57.573 | 77.686 | 1.00 | 31.70 | 8 | 3790 | O | PHE A 480 | 40.568 | 60.548 | 70.019 | 1.00 | 17.08 | 8 |
| 3751 | N | ASN A 474 | 24.396 | 59.107 | 75.308 | 1.00 | 18.40 | 7 | 3791 | CB | PHE A 480 | 38.538 | 57.834 | 69.938 | 1.00 | 14.92 | 6 |
| 3752 | CA | ASN A 474 | 23.632 | 60.348 | 75.444 | 1.00 | 19.45 | 6 | 3792 | CG | PHE A 480 | 37.888 | 58.695 | 68.846 | 1.00 | 15.98 | 6 |
| 3753 | C | ASN A 474 | 24.194 | 61.523 | 74.646 | 1.00 | 19.99 | 6 | 3793 | CD1 | PHE A 480 | 36.748 | 59.437 | 69.087 | 1.00 | 14.48 | 6 |
| 3754 | O | ASN A 474 | 24.363 | 62.658 | 75.103 | 1.00 | 15.86 | 8 | 3794 | CD2 | PHE A 480 | 38.493 | 58.728 | 67.589 | 1.00 | 14.19 | 6 |
| 3755 | CB | ASN A 474 | 23.685 | 60.707 | 76.968 | 1.00 | 22.35 | 6 | 3795 | CE1 | PHE A 480 | 36.160 | 60.227 | 68.092 | 1.00 | 18.16 | 6 |
| 3756 | CG | ASN A 474 | 22.991 | 59.572 | 77.722 | 1.00 | 31.24 | 6 | 3796 | CE2 | PHE A 480 | 37.899 | 59.513 | 66.609 | 1.00 | 18.21 | 6 |
| 3757 | OD1 | ASN A 474 | 22.086 | 58.887 | 77.191 | 1.00 | 32.57 | 8 | 3797 | CZ | PHE A 480 | 36.770 | 60.255 | 66.848 | 1.00 | 19.62 | 6 |
| 3758 | ND2 | ASN A 474 | 23.579 | 59.303 | 78.890 | 1.00 | 32.67 | 7 | 3798 | N | THR A 481 | 41.459 | 58.476 | 69.565 | 1.00 | 15.04 | 7 |
| 3759 | N | GLY A 475 | 24.452 | 61.223 | 73.341 | 1.00 | 17.78 | 7 | 3799 | CA | THR A 481 | 42.525 | 59.036 | 68.696 | 1.00 | 12.66 | 6 |
| 3760 | CA | GLY A 475 | 24.866 | 62.311 | 72.438 | 1.00 | 20.56 | 6 | 3800 | C | THR A 481 | 42.186 | 58.783 | 67.223 | 1.00 | 14.82 | 6 |
| 3761 | C | GLY A 475 | 26.369 | 62.573 | 72.430 | 1.00 | 18.34 | 6 | 3801 | O | THR A 481 | 41.811 | 57.641 | 66.885 | 1.00 | 16.40 | 8 |
| 3762 | O | GLY A 475 | 26.807 | 63.464 | 71.690 | 1.00 | 20.59 | 8 | 3802 | CB | THR A 481 | 43.859 | 58.332 | 69.002 | 1.00 | 19.94 | 6 |
| 3763 | N | SER A 476 | 27.146 | 61.894 | 73.305 | 1.00 | 18.39 | 7 | 3803 | OG1 | THR A 481 | 44.253 | 58.543 | 70.360 | 1.00 | 21.84 | 8 |

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|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 3804 | CG2 | THR | A | 481 | 44.953 | 58.894 | 68.091 | 1.00 | 20.55 | 6 | 3846 | OG | SER | A | 488 | 36.431 | 55.439 | 61.907 | 1.00 | 19.75 | 8 |
| 3805 | N | LEU | A | 482 | 42.216 | 59.860 | 66.454 | 1.00 | 14.98 | 7 | 3847 | N | VAL | A | 489 | 33.950 | 55.975 | 59.626 | 1.00 | 11.85 | 7 |
| 3806 | CA | LEU | A | 482 | 42.004 | 59.690 | 64.991 | 1.00 | 13.06 | 6 | 3848 | CA | VAL | A | 489 | 32.567 | 56.313 | 59.340 | 1.00 | 11.74 | 6 |
| 3807 | C | LEU | A | 482 | 43.383 | 59.527 | 64.394 | 1.00 | 14.32 | 6 | 3849 | C | VAL | A | 489 | 31.685 | 55.457 | 60.269 | 1.00 | 12.51 | 6 |
| 3808 | O | LEU | A | 482 | 44.199 | 60.432 | 64.487 | 1.00 | 15.20 | 8 | 3850 | O | VAL | A | 489 | 31.910 | 54.276 | 60.410 | 1.00 | 13.59 | 8 |
| 3809 | CB | LEU | A | 482 | 41.231 | 60.917 | 64.486 | 1.00 | 13.14 | 6 | 3851 | CB | VAL | A | 489 | 32.231 | 55.903 | 57.882 | 1.00 | 12.50 | 6 |
| 3810 | CG | LEU | A | 482 | 40.812 | 60.936 | 62.999 | 1.00 | 14.96 | 6 | 3852 | CG1 | VAL | A | 489 | 30.712 | 56.154 | 57.650 | 1.00 | 11.14 | 6 |
| 3811 | CD1 | LEU | A | 482 | 39.938 | 59.717 | 62.720 | 1.00 | 16.24 | 6 | 3853 | CG2 | VAL | A | 489 | 32.978 | 56.812 | 56.882 | 1.00 | 13.14 | 6 |
| 3812 | CD2 | LEU | A | 482 | 40.073 | 62.242 | 62.727 | 1.00 | 14.36 | 6 | 3854 | N | TRP | A | 490 | 30.771 | 56.135 | 60.914 | 1.00 | 11.35 | 7 |
| 3813 | N | ALA | A | 483 | 43.621 | 58.414 | 63.680 | 1.00 | 12.65 | 7 | 3855 | CA | TRP | A | 490 | 29.900 | 55.413 | 61.883 | 1.00 | 11.90 | 6 |
| 3814 | CA | ALA | A | 483 | 44.961 | 58.090 | 63.175 | 1.00 | 13.54 | 6 | 3856 | C | TRP | A | 490 | 28.446 | 55.715 | 61.508 | 1.00 | 13.16 | 6 |
| 3815 | C | ALA | A | 483 | 45.370 | 58.961 | 62.000 | 1.00 | 13.15 | 6 | 3857 | O | TRP | A | 490 | 28.103 | 56.878 | 61.324 | 1.00 | 16.40 | 8 |
| 3816 | O | ALA | A | 483 | 44.562 | 59.723 | 61.387 | 1.00 | 13.10 | 8 | 3858 | CB | TRP | A | 490 | 30.222 | 55.953 | 63.283 | 1.00 | 12.61 | 6 |
| 3817 | CB | ALA | A | 483 | 44.892 | 56.581 | 62.782 | 1.00 | 12.82 | 6 | 3859 | CB | TRP | A | 490 | 31.708 | 55.807 | 63.639 | 1.00 | 12.91 | 6 |
| 3818 | N | PRO | A | 484 | 46.637 | 58.980 | 61.687 | 1.00 | 14.66 | 7 | 3860 | CD1 | TRP | A | 490 | 32.381 | 54.628 | 63.904 | 1.00 | 14.71 | 6 |
| 3819 | CA | PRO | A | 484 | 47.183 | 59.827 | 60.632 | 1.00 | 11.27 | 6 | 3861 | CD2 | TRP | A | 490 | 32.632 | 56.884 | 63.716 | 1.00 | 14.18 | 6 |
| 3820 | C | PRO | A | 484 | 46.509 | 59.496 | 59.301 | 1.00 | 12.98 | 6 | 3862 | NE1 | TRP | A | 490 | 33.717 | 54.969 | 64.166 | 1.00 | 13.76 | 7 |
| 3821 | O | PRO | A | 484 | 46.374 | 58.331 | 58.884 | 1.00 | 13.40 | 8 | 3863 | CE2 | TRP | A | 490 | 33.883 | 56.328 | 64.049 | 1.00 | 14.41 | 6 |
| 3822 | CB | PRO | A | 484 | 48.704 | 59.546 | 60.545 | 1.00 | 15.48 | 6 | 3864 | CE3 | TRP | A | 490 | 32.509 | 58.271 | 63.546 | 1.00 | 16.82 | 6 |
| 3823 | CG | PRO | A | 484 | 48.959 | 58.945 | 61.936 | 1.00 | 15.92 | 6 | 3865 | CZ2 | TRP | A | 490 | 35.020 | 57.117 | 64.216 | 1.00 | 13.91 | 6 |
| 3824 | CD | PRO | A | 484 | 47.698 | 58.160 | 62.333 | 1.00 | 15.61 | 6 | 3866 | CZ3 | TRP | A | 490 | 33.641 | 59.052 | 63.701 | 1.00 | 14.61 | 6 |
| 3825 | N | GLY | A | 485 | 45.977 | 60.548 | 58.671 | 1.00 | 14.03 | 7 | 3867 | CH2 | TRP | A | 490 | 34.894 | 58.461 | 64.044 | 1.00 | 14.54 | 6 |
| 3826 | CA | GLY | A | 485 | 45.399 | 60.352 | 57.309 | 1.00 | 13.19 | 6 | 3868 | N | GLN | A | 491 | 27.680 | 54.618 | 61.394 | 1.00 | 11.75 | 7 |
| 3827 | C | GLY | A | 485 | 44.067 | 59.600 | 57.376 | 1.00 | 16.21 | 6 | 3869 | CA | GLN | A | 491 | 26.332 | 54.869 | 60.903 | 1.00 | 12.20 | 6 |
| 3828 | O | GLY | A | 485 | 43.561 | 59.235 | 56.271 | 1.00 | 13.21 | 8 | 3870 | C | GLN | A | 491 | 25.819 | 54.121 | 61.637 | 1.00 | 13.63 | 6 |
| 3829 | N | ALA | A | 486 | 43.508 | 59.349 | 58.553 | 1.00 | 11.65 | 7 | 3871 | O | GLN | A | 491 | 25.472 | 53.092 | 62.207 | 1.00 | 13.45 | 8 |
| 3830 | CA | ALA | A | 486 | 42.375 | 58.395 | 58.545 | 1.00 | 13.98 | 6 | 3872 | CB | GLN | A | 491 | 26.259 | 54.452 | 59.410 | 1.00 | 12.17 | 6 |
| 3831 | C | ALA | A | 486 | 41.058 | 58.969 | 58.068 | 1.00 | 15.41 | 6 | 3873 | CG | GLN | A | 491 | 26.541 | 52.972 | 59.117 | 1.00 | 12.78 | 6 |
| 3832 | O | ALA | A | 486 | 40.730 | 60.148 | 58.196 | 1.00 | 13.33 | 8 | 3874 | CD | GLN | A | 491 | 25.208 | 52.219 | 58.993 | 1.00 | 19.79 | 6 |
| 3833 | CB | ALA | A | 486 | 42.233 | 57.937 | 60.002 | 1.00 | 14.43 | 6 | 3875 | OE1 | GLN | A | 491 | 24.222 | 52.726 | 58.485 | 1.00 | 16.61 | 8 |
| 3834 | N | VAL | A | 487 | 40.213 | 58.008 | 57.647 | 1.00 | 12.17 | 7 | 3876 | NE2 | GLN | A | 491 | 25.214 | 50.952 | 59.455 | 1.00 | 19.28 | 7 |
| 3835 | CA | VAL | A | 487 | 38.776 | 58.220 | 57.403 | 1.00 | 9.79 | 6 | 3877 | N | TYR | A | 492 | 24.024 | 54.698 | 61.523 | 1.00 | 13.67 | 7 |
| 3836 | C | VAL | A | 487 | 38.057 | 57.174 | 58.257 | 1.00 | 9.96 | 6 | 3878 | CA | TYR | A | 492 | 22.819 | 54.043 | 62.092 | 1.00 | 14.21 | 6 |
| 3837 | O | VAL | A | 487 | 38.406 | 55.970 | 58.179 | 1.00 | 12.30 | 8 | 3879 | C | TYR | A | 492 | 21.665 | 54.203 | 61.102 | 1.00 | 17.30 | 6 |
| 3838 | CB | VAL | A | 487 | 38.428 | 58.022 | 55.919 | 1.00 | 10.95 | 6 | 3880 | O | TYR | A | 492 | 21.507 | 55.341 | 60.614 | 1.00 | 14.76 | 8 |
| 3839 | CG1 | VAL | A | 487 | 36.871 | 58.150 | 55.762 | 1.00 | 12.89 | 6 | 3881 | CB | TYR | A | 492 | 22.452 | 54.774 | 63.393 | 1.00 | 15.27 | 6 |
| 3840 | CG2 | VAL | A | 487 | 39.127 | 58.990 | 54.964 | 1.00 | 15.13 | 6 | 3882 | CG | TYR | A | 492 | 21.152 | 54.219 | 63.984 | 1.00 | 15.56 | 6 |
| 3841 | N | SER | A | 488 | 37.112 | 57.635 | 59.078 | 1.00 | 11.84 | 7 | 3883 | CD1 | TYR | A | 492 | 21.146 | 53.010 | 64.638 | 1.00 | 20.95 | 6 |
| 3842 | CA | SER | A | 488 | 36.335 | 56.623 | 59.865 | 1.00 | 12.18 | 6 | 3884 | CD2 | TYR | A | 492 | 19.963 | 54.959 | 63.800 | 1.00 | 18.48 | 6 |
| 3843 | C | SER | A | 488 | 34.867 | 56.972 | 59.659 | 1.00 | 11.64 | 6 | 3885 | CE1 | TYR | A | 492 | 19.956 | 52.511 | 65.176 | 1.00 | 21.55 | 6 |
| 3844 | O | SER | A | 488 | 34.519 | 58.154 | 59.650 | 1.00 | 12.81 | 8 | 3886 | CE2 | TYR | A | 492 | 18.770 | 54.444 | 64.324 | 1.00 | 19.51 | 6 |
| 3845 | CB | SER | A | 488 | 36.850 | 56.705 | 61.336 | 1.00 | 15.82 | 6 | 3887 | CZ | TYR | A | 492 | 18.817 | 53.254 | 65.003 | 1.00 | 22.52 | 6 |

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|------|-----|------------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3888 | OH | TYR A 492 | 17.596 | 52.781 | 65.511 | 1.00 | 24.89 | 8 | 3928 | CB | PRO A 499 | 4.930 | 59.294 | 54.823 | 1.00 | 20.07 | 6 |
| 3889 | N | SER A 493 | 20.879 | 53.151 | 60.925 | 1.00 | 15.17 | 7 | 3929 | CG | PRO A 499 | 3.927 | 59.790 | 55.829 | 1.00 | 23.72 | 6 |
| 3890 | CA | SER A 493 | 19.666 | 53.363 | 60.096 | 1.00 | 14.91 | 6 | 3930 | CD | PRO A 499 | 4.205 | 59.113 | 57.173 | 1.00 | 23.70 | 6 |
| 3891 | C | SER A 493 | 18.548 | 52.462 | 60.616 | 1.00 | 20.17 | 6 | 3931 | N | GLN A 500 | 8.288 | 59.975 | 55.037 | 1.00 | 18.24 | 7 |
| 3892 | O | SER A 493 | 18.887 | 51.457 | 61.255 | 1.00 | 22.90 | 8 | 3932 | CA | GLN A 500 | 9.423 | 60.939 | 55.075 | 1.00 | 13.65 | 6 |
| 3893 | CB | SER A 493 | 19.867 | 53.083 | 58.619 | 1.00 | 23.97 | 6 | 3933 | C | GLN A 500 | 9.921 | 61.084 | 53.596 | 1.00 | 12.93 | 6 |
| 3894 | OG | SER A 493 | 20.148 | 51.710 | 58.532 | 1.00 | 30.62 | 8 | 3934 | O | GLN A 500 | 10.256 | 60.065 | 53.014 | 1.00 | 15.78 | 8 |
| 3895 | N | THR A 494 | 17.344 | 52.991 | 60.393 | 1.00 | 15.89 | 7 | 3935 | CB | GLN A 500 | 10.601 | 60.286 | 55.860 | 1.00 | 15.18 | 6 |
| 3896 | CA | THR A 494 | 16.243 | 52.127 | 60.906 | 1.00 | 18.40 | 6 | 3936 | CG | GLN A 500 | 10.189 | 60.048 | 57.328 | 1.00 | 16.32 | 6 |
| 3897 | C | THR A 494 | 14.999 | 52.406 | 60.060 | 1.00 | 20.14 | 6 | 3937 | CD | GLN A 500 | 11.284 | 59.264 | 58.126 | 1.00 | 15.95 | 6 |
| 3898 | O | THR A 494 | 14.967 | 53.429 | 59.367 | 1.00 | 20.45 | 8 | 3938 | OE1 | GLN A 500 | 12.239 | 58.781 | 57.571 | 1.00 | 17.99 | 8 |
| 3899 | CB | THR A 494 | 15.993 | 52.424 | 62.336 | 1.00 | 24.38 | 6 | 3939 | NE2 | GLN A 500 | 11.008 | 59.238 | 59.419 | 1.00 | 20.52 | 7 |
| 3900 | OG1 | THR A 494 | 15.137 | 51.363 | 62.864 | 1.00 | 25.66 | 8 | 3940 | N | ILE A 501 | 9.662 | 62.283 | 53.054 | 1.00 | 12.81 | 7 |
| 3901 | CG2 | THR A 494 | 15.368 | 53.751 | 62.737 | 1.00 | 27.09 | 6 | 3941 | CA | ILE A 501 | 10.101 | 62.501 | 51.667 | 1.00 | 12.56 | 6 |
| 3902 | N | SER A 495 | 14.017 | 51.534 | 60.157 | 1.00 | 22.56 | 7 | 3942 | C | ILE A 501 | 11.594 | 62.914 | 51.642 | 1.00 | 13.47 | 6 |
| 3903 | CA | SER A 495 | 12.772 | 51.870 | 59.422 | 1.00 | 19.72 | 6 | 3943 | O | ILE A 501 | 11.899 | 63.905 | 52.301 | 1.00 | 14.35 | 8 |
| 3904 | C | SER A 495 | 12.082 | 53.049 | 60.021 | 1.00 | 19.50 | 6 | 3944 | CB | ILE A 501 | 9.262 | 63.635 | 51.032 | 1.00 | 12.51 | 6 |
| 3905 | O | SER A 495 | 12.132 | 53.418 | 61.188 | 1.00 | 21.11 | 8 | 3945 | CG1 | ILE A 501 | 7.788 | 63.216 | 50.842 | 1.00 | 14.81 | 6 |
| 3906 | CB | ASER A 495 | 11.766 | 50.698 | 59.444 | 0.60 | 26.59 | 6 | 3946 | CG2 | ILE A 501 | 9.888 | 63.939 | 49.629 | 1.00 | 12.71 | 6 |
| 3907 | OG | ASER A 495 | 12.447 | 49.487 | 59.259 | 0.60 | 31.40 | 8 | 3947 | CD1 | ILE A 501 | 6.897 | 64.308 | 50.244 | 1.00 | 15.70 | 6 |
| 3908 | CB | BSE A 495 | 11.888 | 50.603 | 59.441 | 0.40 | 20.10 | 6 | 3948 | N | GLY A 502 | 12.383 | 62.169 | 50.872 | 1.00 | 12.33 | 7 |
| 3909 | OG | BSE A 495 | 11.922 | 50.184 | 60.798 | 0.40 | 20.04 | 8 | 3949 | CA | GLY A 502 | 13.793 | 62.673 | 50.746 | 1.00 | 12.41 | 6 |
| 3910 | N | ALA A 496 | 11.315 | 53.727 | 59.141 | 1.00 | 20.53 | 7 | 3950 | C | GLY A 502 | 13.915 | 63.416 | 49.403 | 1.00 | 11.68 | 6 |
| 3911 | C | ALA A 496 | 10.529 | 54.893 | 59.493 | 1.00 | 21.55 | 6 | 3951 | O | GLY A 502 | 14.806 | 64.300 | 49.332 | 1.00 | 12.18 | 8 |
| 3912 | CB | ALA A 496 | 9.094 | 54.492 | 59.960 | 1.00 | 24.11 | 6 | 3952 | N | SER A 503 | 13.120 | 63.068 | 48.395 | 1.00 | 12.99 | 7 |
| 3913 | N | SER A 497 | 8.536 | 53.596 | 59.350 | 1.00 | 29.93 | 8 | 3953 | CA | SER A 503 | 13.334 | 63.710 | 47.073 | 1.00 | 12.73 | 6 |
| 3914 | CA | SER A 497 | 10.354 | 55.717 | 58.189 | 1.00 | 22.92 | 6 | 3954 | C | SER A 503 | 11.970 | 63.672 | 46.342 | 1.00 | 14.01 | 6 |
| 3915 | C | SER A 497 | 7.226 | 54.967 | 61.354 | 1.00 | 26.84 | 7 | 3955 | O | SER A 503 | 11.263 | 62.678 | 46.449 | 1.00 | 14.22 | 8 |
| 3916 | O | SER A 497 | 6.242 | 56.009 | 60.853 | 1.00 | 31.20 | 6 | 3956 | CB | SER A 503 | 14.364 | 62.853 | 46.296 | 1.00 | 12.66 | 6 |
| 3917 | CB | SER A 497 | 7.183 | 54.836 | 62.875 | 1.00 | 35.13 | 6 | 3957 | OG | SER A 503 | 14.467 | 63.267 | 44.940 | 1.00 | 12.94 | 8 |
| 3918 | OG | SER A 497 | 7.578 | 56.030 | 63.515 | 1.00 | 39.06 | 8 | 3958 | N | VAL A 504 | 11.736 | 64.763 | 45.625 | 1.00 | 12.13 | 7 |
| 3919 | N | ALA A 498 | 6.685 | 56.920 | 59.967 | 1.00 | 25.21 | 7 | 3959 | CA | VAL A 504 | 10.738 | 64.716 | 44.521 | 1.00 | 11.27 | 6 |
| 3920 | CA | ALA A 498 | 5.749 | 57.878 | 59.354 | 1.00 | 21.05 | 6 | 3960 | C | VAL A 504 | 11.521 | 65.159 | 43.243 | 1.00 | 11.68 | 6 |
| 3921 | C | ALA A 498 | 6.350 | 58.189 | 57.975 | 1.00 | 22.00 | 6 | 3961 | O | VAL A 504 | 12.287 | 66.121 | 43.321 | 1.00 | 11.43 | 8 |
| 3922 | O | ALA A 498 | 7.541 | 57.907 | 57.763 | 1.00 | 18.25 | 8 | 3962 | CB | VAL A 504 | 9.614 | 65.700 | 44.790 | 1.00 | 12.52 | 6 |
| 3923 | CB | ALA A 498 | 5.737 | 59.103 | 60.231 | 1.00 | 22.15 | 6 | 3963 | CG1 | VAL A 504 | 8.670 | 65.765 | 43.563 | 1.00 | 15.49 | 6 |
| 3924 | N | PRO A 499 | 5.633 | 58.771 | 57.054 | 1.00 | 18.84 | 7 | 3964 | CG2 | VAL A 504 | 8.740 | 65.263 | 46.021 | 1.00 | 12.38 | 6 |
| 3925 | CA | PRO A 499 | 6.176 | 59.058 | 55.718 | 1.00 | 19.31 | 6 | 3965 | N | ALA A 505 | 11.424 | 64.285 | 42.236 | 1.00 | 11.00 | 7 |
| 3926 | C | PRO A 499 | 7.174 | 60.210 | 55.762 | 1.00 | 15.69 | 6 | 3966 | CA | ALA A 505 | 12.174 | 64.595 | 41.003 | 1.00 | 10.56 | 6 |
| 3927 | O | PRO A 499 | 6.934 | 61.242 | 56.370 | 1.00 | 16.96 | 8 | 3967 | C | ALA A 505 | 11.447 | 64.174 | 39.798 | 1.00 | 12.28 | 6 |
| | | | | | | | | | 3968 | O | ALA A 505 | 10.738 | 63.165 | 39.919 | 1.00 | 13.54 | 8 |
| | | | | | | | | | 3969 | CB | ALA A 505 | 13.567 | 63.894 | 41.072 | 1.00 | 11.90 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|---|
| 3970 | N | PRO A 506 | 11.674 | 64.766 | 38.661 | 1.00 | 12.95 | 7 | 4012 | N | GLY A 512 | 0.462 | 65.892 | 33.876 | 1.00 | 12.55 | 7 |
| 3971 | CA | PRO A 506 | 12.353 | 66.020 | 38.410 | 1.00 | 11.12 | 6 | 4013 | CA | GLY A 512 | 0.554 | 64.629 | 33.165 | 1.00 | 14.21 | 6 |
| 3972 | C | PRO A 506 | 11.747 | 67.182 | 39.194 | 1.00 | 12.55 | 6 | 4014 | C | GLY A 512 | 1.950 | 63.971 | 32.170 | 1.00 | 13.76 | 6 |
| 3973 | O | PRO A 506 | 10.711 | 67.015 | 39.862 | 1.00 | 12.33 | 8 | 4015 | O | GLY A 512 | 2.002 | 62.765 | 32.923 | 1.00 | 15.31 | 8 |
| 3974 | CB | PRO A 506 | 12.227 | 66.313 | 36.887 | 1.00 | 13.30 | 6 | 4016 | N | ASN A 513 | 2.994 | 64.789 | 33.454 | 1.00 | 12.18 | 7 |
| 3975 | CG | PRO A 506 | 11.545 | 65.090 | 36.310 | 1.00 | 15.76 | 6 | 4017 | CA | ASN A 513 | 4.306 | 64.154 | 33.561 | 1.00 | 10.79 | 6 |
| 3976 | CD | PRO A 506 | 11.007 | 64.329 | 37.471 | 1.00 | 14.19 | 6 | 4018 | C | ASN A 513 | 4.360 | 63.144 | 34.731 | 1.00 | 15.27 | 6 |
| 3977 | N | ASN A 507 | 12.364 | 68.381 | 39.142 | 1.00 | 10.92 | 7 | 4019 | O | ASN A 513 | 3.699 | 63.392 | 35.738 | 1.00 | 13.64 | 8 |
| 3978 | CA | ASN A 507 | 11.835 | 69.493 | 39.909 | 1.00 | 11.12 | 6 | 4020 | CB | ASN A 513 | 5.408 | 65.230 | 33.833 | 1.00 | 11.43 | 6 |
| 3979 | C | ASN A 507 | 10.940 | 70.447 | 39.087 | 1.00 | 10.54 | 6 | 4021 | CG | ASN A 513 | 5.762 | 66.023 | 32.583 | 1.00 | 11.94 | 6 |
| 3980 | O | ASN A 507 | 10.497 | 71.416 | 39.701 | 1.00 | 12.30 | 8 | 4022 | OD1 | ASN A 513 | 6.738 | 66.874 | 32.746 | 1.00 | 16.21 | 8 |
| 3981 | CB | ASN A 507 | 13.043 | 70.353 | 40.401 | 1.00 | 11.79 | 6 | 4023 | ND2 | ASN A 513 | 5.078 | 65.931 | 31.505 | 1.00 | 8.90 | 7 |
| 3982 | CG | ASN A 507 | 14.033 | 69.459 | 41.196 | 1.00 | 14.07 | 6 | 4024 | N | VAL A 514 | 5.280 | 62.177 | 34.576 | 1.00 | 11.74 | 7 |
| 3983 | OD1 | ASN A 507 | 15.192 | 69.361 | 40.778 | 1.00 | 13.37 | 8 | 4025 | CA | VAL A 514 | 5.505 | 61.269 | 35.745 | 1.00 | 11.63 | 6 |
| 3984 | ND2 | ASN A 507 | 13.592 | 68.845 | 42.261 | 1.00 | 13.47 | 7 | 4026 | C | VAL A 514 | 6.594 | 61.894 | 36.612 | 1.00 | 13.73 | 6 |
| 3985 | N | MET A 508 | 10.654 | 70.046 | 37.850 | 1.00 | 10.20 | 7 | 4027 | O | VAL A 514 | 7.617 | 62.379 | 36.131 | 1.00 | 15.35 | 8 |
| 3986 | CA | MET A 508 | 9.823 | 70.957 | 37.021 | 1.00 | 11.04 | 6 | 4028 | CB | VAL A 514 | 6.072 | 59.931 | 35.221 | 1.00 | 13.67 | 6 |
| 3987 | C | MET A 508 | 9.102 | 70.087 | 36.027 | 1.00 | 11.63 | 6 | 4029 | CG1 | VAL A 514 | 6.529 | 59.036 | 36.390 | 1.00 | 14.35 | 6 |
| 3988 | O | MET A 508 | 9.633 | 69.029 | 35.633 | 1.00 | 12.66 | 8 | 4030 | CG2 | VAL A 514 | 5.042 | 59.176 | 34.393 | 1.00 | 16.73 | 6 |
| 3989 | CB | MET A 508 | 10.929 | 71.782 | 36.219 | 1.00 | 12.80 | 6 | 4031 | N | VAL A 515 | 6.335 | 61.959 | 37.923 | 1.00 | 10.41 | 7 |
| 3990 | CG | MET A 508 | 10.270 | 72.808 | 35.305 | 1.00 | 15.57 | 6 | 4032 | CA | VAL A 515 | 7.256 | 62.496 | 38.927 | 1.00 | 12.67 | 6 |
| 3991 | SD | MET A 508 | 11.558 | 73.692 | 34.325 | 1.00 | 12.60 | 16 | 4033 | C | VAL A 515 | 7.433 | 61.442 | 40.001 | 1.00 | 13.31 | 6 |
| 3992 | CE | MET A 508 | 11.921 | 72.582 | 33.003 | 1.00 | 11.82 | 6 | 4034 | O | VAL A 515 | 6.495 | 60.711 | 40.306 | 1.00 | 14.78 | 8 |
| 3993 | N | GLY A 509 | 7.935 | 70.545 | 35.550 | 1.00 | 11.36 | 7 | 4035 | CB | VAL A 515 | 6.563 | 63.772 | 39.511 | 1.00 | 14.30 | 6 |
| 3994 | CA | GLY A 509 | 7.253 | 69.739 | 34.528 | 1.00 | 10.02 | 6 | 4036 | CG1 | VAL A 515 | 7.228 | 64.271 | 40.775 | 1.00 | 18.11 | 6 |
| 3995 | C | GLY A 509 | 5.851 | 70.331 | 34.276 | 1.00 | 13.18 | 6 | 4037 | CG2 | VAL A 515 | 6.678 | 64.883 | 38.435 | 1.00 | 16.90 | 6 |
| 3996 | O | GLY A 509 | 5.506 | 71.321 | 34.889 | 1.00 | 13.82 | 8 | 4038 | N | THR A 516 | 8.669 | 61.321 | 40.514 | 1.00 | 11.19 | 7 |
| 3997 | N | ILE A 510 | 5.070 | 69.599 | 33.480 | 1.00 | 11.23 | 7 | 4039 | CA | THR A 516 | 8.900 | 60.252 | 41.495 | 1.00 | 11.78 | 6 |
| 3998 | CA | ILE A 510 | 3.674 | 70.061 | 33.192 | 1.00 | 12.19 | 6 | 4040 | C | THR A 516 | 9.271 | 60.860 | 42.835 | 1.00 | 11.71 | 6 |
| 3999 | C | ILE A 510 | 2.746 | 68.964 | 33.701 | 1.00 | 11.61 | 6 | 4041 | O | THR A 516 | 10.092 | 61.763 | 42.959 | 1.00 | 12.89 | 8 |
| 4000 | O | ILE A 510 | 3.156 | 67.806 | 33.903 | 1.00 | 13.58 | 8 | 4042 | CB | THR A 516 | 10.107 | 59.384 | 41.001 | 1.00 | 14.88 | 6 |
| 4001 | CB | ILE A 510 | 3.456 | 70.272 | 31.683 | 1.00 | 12.75 | 6 | 4043 | CG1 | THR A 516 | 9.696 | 58.789 | 39.742 | 1.00 | 14.59 | 8 |
| 4002 | CG1 | ILE A 510 | 3.840 | 69.011 | 30.868 | 1.00 | 11.82 | 6 | 4044 | CG2 | THR A 516 | 10.446 | 58.275 | 42.004 | 1.00 | 14.18 | 6 |
| 4003 | CG2 | ILE A 510 | 4.241 | 71.485 | 31.163 | 1.00 | 14.82 | 6 | 4045 | N | ILE A 517 | 8.600 | 60.281 | 43.863 | 1.00 | 9.66 | 7 |
| 4004 | CD1 | ILE A 510 | 3.293 | 69.108 | 29.417 | 1.00 | 18.53 | 6 | 4046 | CA | ILE A 517 | 8.878 | 60.681 | 45.251 | 1.00 | 10.17 | 6 |
| 4005 | N | PRO A 511 | 1.462 | 69.267 | 33.824 | 1.00 | 13.51 | 7 | 4047 | C | ILE A 517 | 9.670 | 59.586 | 45.920 | 1.00 | 13.57 | 6 |
| 4006 | CA | PRO A 511 | 0.442 | 68.291 | 34.164 | 1.00 | 14.15 | 6 | 4048 | O | ILE A 517 | 9.172 | 58.427 | 45.949 | 1.00 | 13.82 | 8 |
| 4007 | C | PRO A 511 | 0.531 | 67.082 | 33.263 | 1.00 | 13.29 | 6 | 4049 | CB | ILE A 517 | 7.493 | 60.899 | 45.948 | 1.00 | 12.16 | 6 |
| 4008 | O | PRO A 511 | 0.780 | 67.180 | 32.026 | 1.00 | 13.86 | 8 | 4050 | CG1 | ILE A 517 | 6.659 | 61.984 | 45.278 | 1.00 | 15.38 | 6 |
| 4009 | CB | PRO A 511 | -0.913 | 69.037 | 33.810 | 1.00 | 13.10 | 6 | 4051 | CG2 | ILE A 517 | 7.745 | 61.419 | 47.392 | 1.00 | 14.69 | 6 |
| 4010 | CG | PRO A 511 | -0.528 | 70.435 | 34.265 | 1.00 | 15.94 | 6 | 4052 | CD1 | ILE A 517 | 5.200 | 61.951 | 45.779 | 1.00 | 22.16 | 6 |
| 4011 | CD | PRO A 511 | 0.925 | 70.625 | 33.729 | 1.00 | 16.03 | 6 | 4053 | N | ASP A 518 | 10.911 | 59.861 | 46.363 | 1.00 | 13.29 | 7 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4054 | CA | ASP A 518 | 11.743 | 58.802 | 46.976 | 1.00 | 14.12 | 6 | 4096 | O | THR A 524 | 1.433 | 48.984 | 49.372 | 1.00 | 34.03 | 8 |
| 4055 | C | ASP A 518 | 11.868 | 59.161 | 48.435 | 1.00 | 13.11 | 6 | 4097 | CB | THR A 524 | 3.314 | 47.505 | 51.308 | 1.00 | 36.63 | 6 |
| 4056 | O | ASP A 518 | 11.922 | 60.347 | 48.791 | 1.00 | 14.37 | 8 | 4098 | OG1 | THR A 524 | 2.403 | 47.020 | 52.315 | 1.00 | 34.71 | 8 |
| 4057 | CB | ASP A 518 | 13.159 | 58.791 | 46.351 | 1.00 | 14.49 | 6 | 4099 | CG2 | THR A 524 | 4.711 | 47.251 | 51.862 | 1.00 | 34.40 | 6 |
| 4058 | CG | ASP A 518 | 13.106 | 58.207 | 44.962 | 1.00 | 17.62 | 6 | 4100 | N | THR A 525 | 0.748 | 49.673 | 51.432 | 1.00 | 27.38 | 7 |
| 4059 | OD1 | ASP A 518 | 12.858 | 56.963 | 44.888 | 1.00 | 17.47 | 8 | 4101 | CA | THR A 525 | -0.646 | 49.948 | 51.027 | 1.00 | 29.73 | 6 |
| 4060 | OD2 | ASP A 518 | 13.289 | 58.874 | 43.931 | 1.00 | 16.96 | 8 | 4102 | C | THR A 525 | -0.696 | 51.367 | 50.456 | 1.00 | 29.44 | 6 |
| 4061 | N | GLY A 519 | 11.769 | 58.138 | 49.315 | 1.00 | 13.39 | 7 | 4103 | O | THR A 525 | -0.315 | 52.313 | 51.159 | 1.00 | 28.46 | 8 |
| 4062 | CA | GLY A 519 | 11.872 | 58.484 | 50.757 | 1.00 | 14.21 | 6 | 4104 | CB | THR A 525 | -1.558 | 49.835 | 52.265 | 1.00 | 31.59 | 6 |
| 4063 | C | GLY A 519 | 11.716 | 57.152 | 51.549 | 1.00 | 13.61 | 6 | 4105 | OG1 | THR A 525 | -1.416 | 48.485 | 52.779 | 1.00 | 34.50 | 8 |
| 4064 | O | GLY A 519 | 12.278 | 56.130 | 51.134 | 1.00 | 15.70 | 8 | 4106 | CG2 | THR A 525 | -3.020 | 50.076 | 51.920 | 1.00 | 33.53 | 6 |
| 4065 | N | LYS A 520 | 11.059 | 57.319 | 52.696 | 1.00 | 17.22 | 7 | 4107 | N | GLN A 526 | -1.341 | 51.530 | 49.304 | 1.00 | 26.38 | 7 |
| 4066 | CA | LYS A 520 | 10.867 | 56.091 | 53.545 | 1.00 | 15.85 | 6 | 4108 | CA | GLN A 526 | -1.383 | 52.864 | 48.695 | 1.00 | 27.25 | 6 |
| 4067 | C | LYS A 520 | 9.539 | 56.230 | 54.256 | 1.00 | 16.54 | 6 | 4109 | C | GLN A 526 | -2.090 | 53.867 | 49.574 | 1.00 | 29.32 | 6 |
| 4068 | O | LYS A 520 | 9.004 | 57.334 | 54.385 | 1.00 | 17.43 | 8 | 4110 | O | GLN A 526 | -3.264 | 53.665 | 49.960 | 1.00 | 25.61 | 8 |
| 4069 | CB | LYS A 520 | 11.866 | 56.344 | 54.747 | 1.00 | 17.75 | 6 | 4111 | CB | GLN A 526 | -2.101 | 52.757 | 47.340 | 1.00 | 28.17 | 6 |
| 4070 | CG | LYS A 520 | 13.318 | 56.307 | 54.421 | 1.00 | 24.98 | 6 | 4112 | CG | GLN A 526 | -2.028 | 53.996 | 46.486 | 1.00 | 30.46 | 6 |
| 4071 | CD | LYS A 520 | 14.147 | 56.512 | 55.698 | 1.00 | 22.21 | 6 | 4113 | CD | GLN A 526 | -2.542 | 53.744 | 45.055 | 1.00 | 28.73 | 6 |
| 4072 | CE | LYS A 520 | 14.074 | 55.145 | 56.459 | 1.00 | 23.54 | 6 | 4114 | OE1 | GLN A 526 | -3.419 | 54.518 | 44.679 | 1.00 | 33.21 | 8 |
| 4073 | NZ | LYS A 520 | 15.426 | 54.879 | 57.005 | 1.00 | 27.08 | 7 | 4115 | NE2 | GLN A 526 | -1.951 | 52.750 | 44.438 | 1.00 | 31.17 | 7 |
| 4074 | CA | GLY A 521 | 9.021 | 55.065 | 54.728 | 1.00 | 16.42 | 7 | 4116 | N | GLY A 527 | -1.476 | 55.032 | 49.820 | 1.00 | 22.05 | 7 |
| 4075 | N | GLY A 521 | 7.870 | 55.223 | 55.627 | 1.00 | 16.98 | 6 | 4117 | CA | GLY A 527 | -2.091 | 56.150 | 50.508 | 1.00 | 20.00 | 6 |
| 4076 | C | GLY A 521 | 6.540 | 55.347 | 54.874 | 1.00 | 19.49 | 6 | 4118 | C | GLY A 527 | -2.415 | 57.258 | 49.471 | 1.00 | 19.58 | 6 |
| 4077 | O | GLY A 521 | 5.533 | 55.716 | 55.525 | 1.00 | 18.22 | 8 | 4119 | O | GLY A 527 | -2.894 | 56.897 | 48.405 | 1.00 | 21.95 | 8 |
| 4078 | N | PHE A 522 | 6.569 | 55.053 | 53.560 | 1.00 | 19.15 | 7 | 4120 | N | THR A 528 | -2.136 | 58.506 | 49.804 | 1.00 | 21.30 | 7 |
| 4079 | CA | PHE A 522 | 5.299 | 55.230 | 52.839 | 1.00 | 17.53 | 6 | 4121 | CA | THR A 528 | -2.428 | 59.597 | 48.884 | 1.00 | 18.42 | 6 |
| 4080 | C | PHE A 522 | 4.344 | 54.037 | 53.029 | 1.00 | 20.57 | 6 | 4122 | C | THR A 528 | -1.268 | 60.584 | 48.808 | 1.00 | 21.48 | 6 |
| 4081 | O | PHE A 522 | 3.173 | 54.222 | 52.638 | 1.00 | 20.45 | 8 | 4123 | O | THR A 528 | -0.375 | 60.642 | 49.647 | 1.00 | 20.31 | 8 |
| 4082 | CB | PHE A 522 | 5.587 | 55.448 | 51.342 | 1.00 | 17.55 | 6 | 4124 | CB | THR A 528 | -3.685 | 60.387 | 49.320 | 1.00 | 24.98 | 6 |
| 4083 | CG | PHE A 522 | 6.513 | 56.605 | 51.009 | 1.00 | 15.40 | 6 | 4125 | OG1 | THR A 528 | -3.522 | 60.782 | 50.657 | 1.00 | 30.73 | 8 |
| 4084 | CD1 | PHE A 522 | 6.601 | 57.740 | 51.763 | 1.00 | 17.48 | 6 | 4126 | CG2 | THR A 528 | -4.933 | 59.511 | 49.240 | 1.00 | 26.25 | 6 |
| 4085 | CD2 | PHE A 522 | 7.262 | 56.452 | 49.824 | 1.00 | 17.80 | 6 | 4127 | N | VAL A 529 | -1.209 | 61.255 | 47.667 | 1.00 | 16.67 | 7 |
| 4086 | CE1 | PHE A 522 | 7.480 | 58.778 | 51.376 | 1.00 | 20.21 | 6 | 4128 | CA | VAL A 529 | -0.167 | 62.275 | 47.425 | 1.00 | 15.19 | 6 |
| 4087 | CE2 | PHE A 522 | 8.142 | 57.475 | 49.422 | 1.00 | 16.35 | 6 | 4129 | C | VAL A 529 | -0.924 | 63.532 | 46.987 | 1.00 | 16.18 | 6 |
| 4088 | CZ | PHE A 522 | 8.257 | 58.607 | 50.214 | 1.00 | 14.66 | 6 | 4130 | O | VAL A 529 | -1.825 | 63.328 | 46.155 | 1.00 | 16.64 | 8 |
| 4089 | N | GLY A 523 | 4.826 | 52.902 | 53.488 | 1.00 | 23.38 | 7 | 4131 | CB | VAL A 529 | 0.700 | 61.851 | 46.216 | 1.00 | 14.16 | 6 |
| 4090 | CA | GLY A 523 | 3.947 | 51.721 | 53.586 | 1.00 | 26.21 | 6 | 4132 | CG1 | VAL A 529 | 1.664 | 62.995 | 45.841 | 1.00 | 17.46 | 6 |
| 4091 | C | GLY A 523 | 3.753 | 51.037 | 52.260 | 1.00 | 27.39 | 6 | 4133 | CG2 | VAL A 529 | 1.483 | 60.594 | 46.604 | 1.00 | 18.23 | 6 |
| 4092 | O | GLY A 523 | 4.082 | 51.536 | 51.167 | 1.00 | 21.64 | 8 | 4134 | N | THR A 530 | -0.533 | 64.669 | 47.531 | 1.00 | 14.50 | 7 |
| 4093 | N | THR A 524 | 3.204 | 49.785 | 52.316 | 1.00 | 26.00 | 7 | 4135 | CA | THR A 530 | -1.148 | 65.900 | 47.016 | 1.00 | 14.78 | 6 |
| 4094 | CA | THR A 524 | 3.043 | 49.010 | 51.103 | 1.00 | 24.30 | 6 | 4136 | C | THR A 530 | -0.038 | 66.814 | 46.492 | 1.00 | 17.57 | 6 |
| 4095 | C | THR A 524 | 1.636 | 49.241 | 50.556 | 1.00 | 26.74 | 6 | 4137 | O | THR A 530 | 1.076 | 66.792 | 47.027 | 1.00 | 15.22 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4138 | CB | THR A 530 | -1.954 | 66.621 | 48.090 | 1.00 | 15.93 | 6 | 4180 | CA | THR A 537 | -3.151 | 60.043 | 40.489 | 1.00 | 15.38 | 6 |
| 4139 | OG1 | THR A 530 | -1.209 | 66.722 | 49.308 | 1.00 | 17.69 | 8 | 4181 | C | THR A 537 | -1.865 | 59.242 | 40.679 | 1.00 | 19.21 | 6 |
| 4140 | CG2 | THR A 530 | -3.279 | 65.858 | 48.340 | 1.00 | 17.39 | 6 | 4182 | O | THR A 537 | -0.823 | 59.697 | 40.166 | 1.00 | 19.02 | 8 |
| 4141 | N | PHE A 531 | -0.395 | 67.691 | 45.569 | 1.00 | 14.04 | 7 | 4183 | CB | THR A 537 | -3.564 | 59.955 | 38.998 | 1.00 | 18.90 | 6 |
| 4142 | CA | PHE A 531 | 0.458 | 68.822 | 45.142 | 1.00 | 13.01 | 6 | 4184 | OG1 | THR A 537 | -4.828 | 60.651 | 38.950 | 1.00 | 19.30 | 8 |
| 4143 | C | PHE A 531 | -0.344 | 70.073 | 45.496 | 1.00 | 15.03 | 6 | 4185 | CG2 | THR A 537 | -3.697 | 58.508 | 38.591 | 1.00 | 18.81 | 6 |
| 4144 | O | PHE A 531 | -1.454 | 70.292 | 44.989 | 1.00 | 16.16 | 8 | 4186 | N | VAL A 538 | -1.925 | 58.176 | 41.415 | 1.00 | 16.51 | 7 |
| 4145 | CB | PHE A 531 | 0.659 | 68.823 | 43.604 | 1.00 | 13.87 | 6 | 4187 | CA | VAL A 538 | -0.704 | 57.394 | 41.746 | 1.00 | 16.38 | 6 |
| 4146 | CG | PHE A 531 | 1.611 | 67.777 | 43.040 | 1.00 | 13.21 | 6 | 4188 | C | VAL A 538 | -0.516 | 56.415 | 40.613 | 1.00 | 18.34 | 6 |
| 4147 | CD1 | PHE A 531 | 1.438 | 66.431 | 43.191 | 1.00 | 14.34 | 6 | 4189 | O | VAL A 538 | -1.390 | 55.599 | 40.252 | 1.00 | 20.80 | 8 |
| 4148 | CD2 | PHE A 531 | 2.662 | 68.228 | 42.240 | 1.00 | 14.96 | 6 | 4190 | CB | VAL A 538 | -0.896 | 56.665 | 43.080 | 1.00 | 17.97 | 6 |
| 4149 | CE1 | PHE A 531 | 2.288 | 65.515 | 42.629 | 1.00 | 16.70 | 6 | 4191 | CG1 | VAL A 538 | -0.219 | 55.621 | 43.337 | 1.00 | 16.03 | 6 |
| 4150 | CE2 | PHE A 531 | 3.545 | 67.306 | 41.691 | 1.00 | 13.81 | 6 | 4192 | CG2 | VAL A 538 | -1.016 | 57.646 | 44.226 | 1.00 | 19.59 | 6 |
| 4151 | CZ | PHE A 531 | 3.385 | 65.943 | 41.836 | 1.00 | 16.70 | 6 | 4193 | N | LVS A 539 | 0.696 | 56.340 | 40.055 | 1.00 | 15.64 | 7 |
| 4152 | N | GLY A 532 | 0.118 | 70.806 | 46.490 | 1.00 | 14.18 | 7 | 4194 | CA | LVS A 539 | 1.119 | 55.341 | 39.108 | 1.00 | 14.97 | 6 |
| 4153 | CA | GLY A 532 | -0.569 | 72.077 | 46.884 | 1.00 | 15.57 | 6 | 4195 | C | LVS A 539 | 1.626 | 54.044 | 39.732 | 1.00 | 17.57 | 6 |
| 4154 | C | GLY A 532 | -1.992 | 71.702 | 47.378 | 1.00 | 19.88 | 6 | 4196 | O | LVS A 539 | 1.313 | 52.885 | 39.375 | 1.00 | 18.05 | 8 |
| 4155 | O | GLY A 532 | -2.928 | 72.482 | 47.068 | 1.00 | 18.91 | 8 | 4197 | CB | LVS A 539 | 2.264 | 55.914 | 38.209 | 1.00 | 17.15 | 6 |
| 4156 | N | GLY A 533 | -2.193 | 70.510 | 47.921 | 1.00 | 17.41 | 7 | 4198 | CG | LVS A 539 | 2.814 | 54.859 | 37.246 | 1.00 | 20.63 | 6 |
| 4157 | CA | GLY A 533 | -3.524 | 70.089 | 48.400 | 1.00 | 18.31 | 6 | 4199 | CD | LVS A 539 | 3.860 | 55.636 | 36.368 | 1.00 | 25.39 | 6 |
| 4158 | C | GLY A 533 | -4.368 | 69.372 | 47.370 | 1.00 | 20.08 | 6 | 4200 | CE | LVS A 539 | 3.601 | 55.199 | 34.949 | 1.00 | 41.98 | 6 |
| 4159 | O | GLY A 533 | -5.463 | 68.817 | 47.637 | 1.00 | 19.31 | 8 | 4201 | NZ | LVS A 539 | 4.369 | 53.976 | 34.672 | 1.00 | 30.47 | 7 |
| 4160 | N | VAL A 534 | -3.923 | 69.391 | 46.097 | 1.00 | 16.06 | 7 | 4202 | N | SER A 540 | 2.424 | 54.212 | 40.787 | 1.00 | 15.53 | 7 |
| 4161 | CA | VAL A 534 | -4.592 | 68.721 | 44.999 | 1.00 | 15.11 | 6 | 4203 | CA | SER A 540 | 2.919 | 53.073 | 41.587 | 1.00 | 16.52 | 6 |
| 4162 | C | VAL A 534 | -4.197 | 67.275 | 44.894 | 1.00 | 15.67 | 6 | 4204 | C | SER A 540 | 3.231 | 53.502 | 42.999 | 1.00 | 17.69 | 6 |
| 4163 | O | VAL A 534 | -3.019 | 66.888 | 44.712 | 1.00 | 17.94 | 8 | 4205 | O | SER A 540 | 3.482 | 54.680 | 43.306 | 1.00 | 16.82 | 8 |
| 4164 | CB | VAL A 534 | -4.368 | 69.480 | 43.645 | 1.00 | 13.67 | 6 | 4206 | CB | SER A 540 | 4.136 | 52.424 | 40.903 | 1.00 | 20.58 | 6 |
| 4165 | CG1 | VAL A 534 | -5.101 | 68.739 | 42.509 | 1.00 | 15.45 | 6 | 4207 | OG | SER A 540 | 5.270 | 53.317 | 41.043 | 1.00 | 19.05 | 8 |
| 4166 | CG2 | VAL A 534 | -4.807 | 70.937 | 43.768 | 1.00 | 13.93 | 7 | 4208 | N | TRP A 541 | 3.206 | 52.536 | 43.953 | 1.00 | 16.64 | 7 |
| 4167 | N | THR A 535 | -5.185 | 66.334 | 44.967 | 1.00 | 16.87 | 6 | 4209 | CA | TRP A 541 | 3.361 | 52.905 | 45.378 | 1.00 | 15.40 | 6 |
| 4168 | CA | THR A 535 | -4.827 | 64.927 | 44.890 | 1.00 | 16.87 | 6 | 4210 | C | TRP A 541 | 4.148 | 51.785 | 46.053 | 1.00 | 20.16 | 6 |
| 4169 | C | THR A 535 | -4.271 | 64.521 | 43.536 | 1.00 | 20.28 | 6 | 4211 | O | TRP A 541 | 3.682 | 50.647 | 46.008 | 1.00 | 21.11 | 8 |
| 4170 | O | THR A 535 | -4.796 | 64.893 | 42.462 | 1.00 | 17.64 | 8 | 4212 | CB | TRP A 541 | 2.034 | 53.084 | 46.101 | 1.00 | 17.49 | 6 |
| 4171 | CB | THR A 535 | -6.065 | 64.042 | 45.192 | 1.00 | 20.23 | 6 | 4213 | CG | TRP A 541 | 2.124 | 53.605 | 47.502 | 1.00 | 15.27 | 6 |
| 4172 | OG1 | THR A 535 | -6.446 | 64.284 | 46.576 | 1.00 | 20.94 | 8 | 4214 | CD1 | TRP A 541 | 2.645 | 52.924 | 48.584 | 1.00 | 18.64 | 6 |
| 4173 | CG2 | THR A 535 | -5.787 | 62.565 | 45.026 | 1.00 | 24.73 | 6 | 4215 | CD2 | TRP A 541 | 1.689 | 54.854 | 48.006 | 1.00 | 15.30 | 6 |
| 4174 | N | ALA A 536 | -3.162 | 63.773 | 43.562 | 1.00 | 15.87 | 7 | 4216 | NE1 | TRP A 541 | 2.542 | 53.673 | 49.715 | 1.00 | 19.85 | 7 |
| 4175 | CA | ALA A 536 | -2.521 | 63.324 | 42.337 | 1.00 | 17.27 | 6 | 4217 | CE2 | TRP A 541 | 1.976 | 54.894 | 47.381 | 1.00 | 17.27 | 6 |
| 4176 | C | ALA A 536 | -2.808 | 61.859 | 42.042 | 1.00 | 20.29 | 6 | 4218 | CE3 | TRP A 541 | 1.086 | 55.984 | 47.440 | 1.00 | 15.92 | 6 |
| 4177 | O | ALA A 536 | -2.929 | 61.111 | 43.030 | 1.00 | 20.32 | 8 | 4219 | CZ2 | TRP A 541 | 1.703 | 55.983 | 50.201 | 1.00 | 18.49 | 6 |
| 4178 | CB | ALA A 536 | -0.976 | 63.441 | 42.384 | 1.00 | 17.03 | 6 | 4220 | CZ3 | TRP A 541 | 0.787 | 57.054 | 48.223 | 1.00 | 19.66 | 6 |
| 4179 | N | THR A 537 | -2.937 | 61.461 | 40.791 | 1.00 | 16.03 | 7 | 4221 | CH2 | TRP A 541 | 1.076 | 57.063 | 49.619 | 1.00 | 21.41 | 8 |

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|------|-----|------------|--------|--------|--------|------|-------|---|------|---------------|-----------|--------|--------|--------|-------|-------|---|
| 4222 | N | THR A 542 | 5.297 | 52.107 | 46.615 | 1.00 | 18.77 | 7 | 4260 | CG2 ILE A 546 | 3.624 | 57.682 | 45.030 | 1.00 | 14.12 | 6 | |
| 4223 | CA | THR A 542 | 6.111 | 51.224 | 47.437 | 1.00 | 20.27 | 6 | 4261 | CD1 ILE A 546 | 4.473 | 57.773 | 48.119 | 1.00 | 13.44 | 6 | |
| 4224 | C | THR A 542 | 6.477 | 51.972 | 48.690 | 1.00 | 21.74 | 6 | 4262 | N | GLU A 547 | 5.424 | 56.777 | 42.400 | 1.00 | 14.74 | 7 |
| 4225 | O | THR A 542 | 6.369 | 53.228 | 48.814 | 1.00 | 17.27 | 8 | 4263 | CA | GLU A 547 | 5.338 | 57.543 | 41.134 | 1.00 | 14.58 | 6 |
| 4226 | CB | THR A 542 | 7.356 | 50.641 | 46.743 | 1.00 | 24.92 | 6 | 4264 | C | GLU A 547 | 3.943 | 58.116 | 40.945 | 1.00 | 15.30 | 6 |
| 4227 | OG1 | THR A 542 | 8.305 | 51.745 | 46.576 | 1.00 | 21.04 | 8 | 4265 | O | GLU A 547 | 2.977 | 57.405 | 41.270 | 1.00 | 15.50 | 8 |
| 4228 | CG2 | THR A 542 | 7.091 | 49.930 | 45.442 | 1.00 | 26.69 | 6 | 4266 | CB | GLU A 547 | 5.537 | 56.644 | 39.913 | 1.00 | 14.75 | 6 |
| 4229 | N | SER A 543 | 7.123 | 51.252 | 49.648 | 1.00 | 18.34 | 7 | 4267 | CG | GLU A 547 | 6.987 | 56.074 | 39.890 | 1.00 | 17.63 | 6 |
| 4230 | CA | SER A 543 | 7.474 | 51.808 | 50.923 | 1.00 | 18.96 | 6 | 4268 | CD | GLU A 547 | 7.105 | 55.058 | 38.781 | 1.00 | 21.54 | 6 |
| 4231 | C | SER A 543 | 8.463 | 52.975 | 50.734 | 1.00 | 17.37 | 6 | 4269 | OE1 | GLU A 547 | 6.335 | 54.046 | 38.730 | 1.00 | 18.28 | 8 |
| 4232 | O | SER A 543 | 8.525 | 53.808 | 51.615 | 1.00 | 19.43 | 8 | 4270 | OE2 | GLU A 547 | 7.924 | 55.225 | 37.834 | 1.00 | 16.92 | 8 |
| 4233 | CB | SER A 543 | 8.201 | 50.711 | 51.743 | 1.00 | 24.79 | 6 | 4271 | N | VAL A 548 | 3.865 | 59.377 | 40.603 | 1.00 | 12.67 | 7 |
| 4234 | OG | SER A 543 | 7.254 | 49.673 | 51.954 | 1.00 | 38.42 | 8 | 4272 | CA | VAL A 548 | 2.565 | 60.033 | 40.428 | 1.00 | 13.16 | 6 |
| 4235 | N | ASN A 544 | 9.313 | 52.865 | 49.721 | 1.00 | 17.78 | 7 | 4273 | C | VAL A 548 | 2.565 | 60.764 | 39.095 | 1.00 | 15.52 | 6 |
| 4236 | CA | ASN A 544 | 10.349 | 53.917 | 49.575 | 1.00 | 14.67 | 6 | 4274 | O | VAL A 548 | 3.587 | 61.028 | 38.477 | 1.00 | 14.55 | 8 |
| 4237 | C | ASN A 544 | 10.208 | 54.723 | 48.287 | 1.00 | 15.24 | 6 | 4275 | CB | VAL A 548 | 2.266 | 61.100 | 41.499 | 1.00 | 15.22 | 6 |
| 4238 | O | ASN A 544 | 11.018 | 55.668 | 48.072 | 1.00 | 16.63 | 8 | 4276 | CG1 | VAL A 548 | 2.134 | 60.409 | 42.872 | 1.00 | 17.06 | 6 |
| 4239 | CB | AASN A 544 | 11.734 | 53.252 | 49.583 | 0.50 | 18.64 | 6 | 4277 | CG2 | VAL A 548 | 3.376 | 62.179 | 41.584 | 1.00 | 16.26 | 6 |
| 4240 | CG | AASN A 544 | 12.145 | 52.868 | 51.005 | 0.50 | 24.93 | 6 | 4278 | N | TYR A 549 | 1.338 | 61.119 | 38.644 | 1.00 | 12.92 | 7 |
| 4241 | OD1 | AASN A 544 | 11.394 | 53.024 | 51.976 | 0.50 | 27.01 | 8 | 4279 | CA | TYR A 549 | 1.226 | 61.997 | 37.481 | 1.00 | 14.43 | 6 |
| 4242 | ND2 | AASN A 544 | 13.359 | 52.364 | 51.118 | 0.50 | 19.54 | 7 | 4280 | C | TYR A 549 | 0.902 | 63.397 | 37.975 | 1.00 | 13.16 | 6 |
| 4240 | CB | BASN A 544 | 11.746 | 53.263 | 49.523 | 0.50 | 15.95 | 6 | 4281 | O | TYR A 549 | 0.223 | 63.571 | 39.016 | 1.00 | 14.84 | 8 |
| 4241 | CG | BASN A 544 | 11.998 | 52.552 | 50.860 | 0.50 | 20.57 | 6 | 4282 | CB | TYR A 549 | 0.000 | 61.611 | 36.605 | 1.00 | 14.89 | 6 |
| 4242 | OD1 | BASN A 544 | 12.195 | 53.205 | 51.884 | 0.50 | 23.06 | 8 | 4283 | CG | TYR A 549 | 0.208 | 60.240 | 36.037 | 1.00 | 14.21 | 6 |
| 4243 | ND2 | BASN A 544 | 11.914 | 51.250 | 50.767 | 0.50 | 19.16 | 7 | 4284 | CD1 | TYR A 549 | 1.049 | 60.058 | 34.934 | 1.00 | 17.04 | 6 |
| 4243 | N | ARG A 545 | 9.224 | 54.409 | 47.426 | 1.00 | 14.40 | 7 | 4285 | CD2 | TYR A 549 | -0.398 | 59.160 | 36.628 | 1.00 | 14.96 | 6 |
| 4244 | CA | ARG A 545 | 9.193 | 55.190 | 46.167 | 1.00 | 16.44 | 6 | 4286 | CE1 | TYR A 549 | 1.252 | 58.788 | 34.395 | 1.00 | 19.51 | 6 |
| 4245 | C | ARG A 545 | 7.727 | 55.246 | 45.682 | 1.00 | 19.39 | 6 | 4287 | CE2 | TYR A 549 | -0.214 | 57.885 | 36.081 | 1.00 | 20.11 | 6 |
| 4246 | O | ARG A 545 | 7.083 | 54.204 | 45.539 | 1.00 | 17.25 | 8 | 4288 | CZ | TYR A 549 | 0.577 | 57.730 | 34.984 | 1.00 | 20.28 | 6 |
| 4247 | CB | ARG A 545 | 10.085 | 54.589 | 45.084 | 1.00 | 17.96 | 6 | 4289 | OH | TYR A 549 | 0.789 | 56.436 | 34.508 | 1.00 | 21.51 | 8 |
| 4248 | CG | ARG A 545 | 9.964 | 55.404 | 43.794 | 1.00 | 17.03 | 6 | 4290 | N | VAL A 550 | 1.626 | 64.446 | 37.496 | 1.00 | 12.41 | 7 |
| 4249 | CD | ARG A 545 | 10.778 | 54.728 | 42.653 | 1.00 | 15.55 | 6 | 4291 | CA | VAL A 550 | 1.317 | 65.794 | 37.957 | 1.00 | 13.30 | 6 |
| 4250 | NE | ARG A 545 | 12.186 | 54.934 | 43.045 | 1.00 | 17.92 | 7 | 4292 | C | VAL A 550 | -0.145 | 66.139 | 37.602 | 1.00 | 12.86 | 6 |
| 4251 | CZ | ARG A 545 | 13.164 | 54.094 | 42.735 | 1.00 | 27.70 | 6 | 4293 | O | VAL A 550 | -0.589 | 65.893 | 36.503 | 1.00 | 15.42 | 8 |
| 4252 | NH1 | ARG A 545 | 12.923 | 53.020 | 41.999 | 1.00 | 26.35 | 7 | 4294 | CB | VAL A 550 | 2.195 | 66.791 | 37.131 | 1.00 | 12.38 | 6 |
| 4253 | NH2 | ARG A 545 | 14.392 | 54.343 | 43.179 | 1.00 | 26.80 | 7 | 4295 | CG1 | VAL A 550 | 1.968 | 68.236 | 37.581 | 1.00 | 13.91 | 6 |
| 4254 | N | ILE A 546 | 7.282 | 56.458 | 45.332 | 1.00 | 18.00 | 7 | 4296 | CG2 | VAL A 550 | 3.657 | 66.404 | 37.542 | 1.00 | 16.31 | 6 |
| 4255 | CA | ILE A 546 | 5.908 | 56.613 | 44.793 | 1.00 | 14.23 | 6 | 4297 | N | PRO A 551 | -0.828 | 66.685 | 38.603 | 1.00 | 13.48 | 7 |
| 4256 | C | ILE A 546 | 6.077 | 57.267 | 43.406 | 1.00 | 17.86 | 6 | 4298 | CA | PRO A 551 | -2.272 | 66.942 | 38.387 | 1.00 | 16.42 | 6 |
| 4257 | O | ILE A 546 | 6.771 | 58.296 | 43.389 | 1.00 | 15.62 | 8 | 4299 | C | PRO A 551 | -2.447 | 68.081 | 37.424 | 1.00 | 16.09 | 6 |
| 4258 | CB | ILE A 546 | 5.039 | 57.498 | 45.668 | 1.00 | 13.38 | 6 | 4300 | O | PRO A 551 | -1.599 | 68.955 | 37.236 | 1.00 | 16.43 | 8 |
| 4259 | CG1 | ILE A 546 | 4.895 | 56.781 | 47.045 | 1.00 | 15.14 | 6 | 4301 | CB | PRO A 551 | -2.869 | 67.337 | 39.755 | 1.00 | 20.53 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4302 | CG | PRO A 551 | -1.772 | 66.991 | 40.707 | 1.00 | 20.55 | 6 | 4344 | C | THR A 558 | 4.469 | 72.927 | 45.741 | 1.00 | 16.19 | 6 |
| 4303 | CD | PRO A 551 | -0.427 | 66.849 | 39.973 | 1.00 | 17.00 | 6 | 4345 | O | THR A 558 | 5.520 | 72.402 | 45.379 | 1.00 | 16.82 | 8 |
| 4304 | N | ASN A 552 | -3.658 | 68.150 | 36.821 | 1.00 | 15.47 | 7 | 4346 | CB | THR A 558 | 2.616 | 73.378 | 44.044 | 1.00 | 17.75 | 6 |
| 4305 | CA | ASN A 552 | -4.017 | 69.248 | 35.941 | 1.00 | 15.18 | 6 | 4347 | OG1 | THR A 558 | 1.566 | 73.153 | 45.010 | 1.00 | 18.46 | 8 |
| 4306 | C | ASN A 552 | -4.401 | 70.475 | 36.748 | 1.00 | 19.54 | 6 | 4348 | CG2 | THR A 558 | 2.886 | 72.099 | 43.320 | 1.00 | 14.65 | 6 |
| 4307 | O | ASN A 552 | -5.630 | 70.744 | 36.917 | 1.00 | 19.65 | 8 | 4349 | N | ASP A 559 | 3.750 | 72.559 | 46.821 | 1.00 | 13.53 | 7 |
| 4308 | CB | ASN A 552 | -5.198 | 68.759 | 35.075 | 1.00 | 19.00 | 6 | 4350 | CA | ASP A 559 | 4.351 | 71.569 | 47.739 | 1.00 | 13.26 | 6 |
| 4309 | CG | ASN A 552 | -5.522 | 69.706 | 33.925 | 1.00 | 23.61 | 6 | 4351 | C | ASP A 559 | 3.718 | 70.202 | 47.564 | 1.00 | 17.40 | 6 |
| 4310 | OD1 | ASN A 552 | -4.763 | 70.583 | 33.553 | 1.00 | 29.14 | 8 | 4352 | O | ASP A 559 | 2.469 | 70.015 | 47.579 | 1.00 | 17.26 | 8 |
| 4311 | ND2 | ASN A 552 | -6.635 | 69.481 | 33.239 | 1.00 | 23.65 | 7 | 4353 | CB | ASP A 559 | 4.129 | 72.027 | 49.195 | 1.00 | 13.77 | 6 |
| 4312 | N | MET A 553 | -3.487 | 71.146 | 37.402 | 1.00 | 13.46 | 7 | 4354 | CG | ASP A 559 | 4.998 | 73.219 | 49.580 | 1.00 | 25.94 | 6 |
| 4313 | CA | MET A 553 | -3.722 | 72.208 | 38.346 | 1.00 | 11.50 | 6 | 4355 | OD1 | ASP A 559 | 6.174 | 73.267 | 49.201 | 1.00 | 23.88 | 8 |
| 4314 | C | MET A 553 | -3.003 | 73.456 | 37.901 | 1.00 | 15.54 | 6 | 4356 | OD2 | ASP A 559 | 4.468 | 74.127 | 50.251 | 1.00 | 28.55 | 8 |
| 4315 | O | MET A 553 | -2.319 | 73.427 | 36.881 | 1.00 | 17.61 | 8 | 4357 | N | VAL A 560 | 4.576 | 69.205 | 47.465 | 1.00 | 12.44 | 7 |
| 4316 | CB | MET A 553 | -3.328 | 71.835 | 39.803 | 1.00 | 16.46 | 6 | 4358 | CA | VAL A 560 | 4.161 | 67.801 | 47.392 | 1.00 | 11.28 | 6 |
| 4317 | CG | MET A 553 | -1.826 | 71.490 | 39.883 | 1.00 | 14.92 | 6 | 4359 | C | VAL A 560 | 4.193 | 67.207 | 48.826 | 1.00 | 14.98 | 6 |
| 4318 | SD | MET A 553 | -1.364 | 70.962 | 41.579 | 1.00 | 17.71 | 16 | 4360 | O | VAL A 560 | 5.085 | 67.470 | 49.616 | 1.00 | 15.44 | 8 |
| 4319 | CE | MET A 553 | -1.416 | 72.450 | 42.426 | 1.00 | 16.59 | 6 | 4361 | CB | VAL A 560 | 5.144 | 66.953 | 46.555 | 1.00 | 11.93 | 6 |
| 4320 | N | ALA A 554 | -3.278 | 74.532 | 38.619 | 1.00 | 17.19 | 7 | 4362 | CG1 | VAL A 560 | 4.738 | 65.496 | 46.488 | 1.00 | 16.58 | 6 |
| 4321 | CA | ALA A 554 | -2.711 | 75.834 | 38.289 | 1.00 | 21.10 | 6 | 4363 | CG2 | VAL A 560 | 5.186 | 67.516 | 45.122 | 1.00 | 14.73 | 6 |
| 4322 | C | ALA A 554 | -1.169 | 75.788 | 38.321 | 1.00 | 17.79 | 6 | 4364 | N | LVS A 561 | 3.136 | 66.439 | 49.097 | 1.00 | 15.49 | 7 |
| 4323 | O | ALA A 554 | -0.631 | 75.032 | 39.141 | 1.00 | 17.24 | 8 | 4365 | CA | LVS A 561 | 2.989 | 65.835 | 50.443 | 1.00 | 14.90 | 6 |
| 4324 | CB | ALA A 554 | -3.075 | 76.757 | 39.471 | 1.00 | 24.10 | 6 | 4366 | C | LVS A 561 | 2.427 | 64.452 | 50.269 | 1.00 | 15.23 | 6 |
| 4325 | N | ALA A 555 | -0.537 | 76.591 | 37.500 | 1.00 | 14.57 | 7 | 4367 | O | LVS A 561 | 1.502 | 64.157 | 49.522 | 1.00 | 16.90 | 8 |
| 4326 | CA | ALA A 555 | 0.947 | 76.567 | 37.489 | 1.00 | 13.27 | 6 | 4368 | CB | LVS A 561 | 1.960 | 66.720 | 51.206 | 1.00 | 18.50 | 6 |
| 4327 | C | ALA A 555 | 1.568 | 77.356 | 38.600 | 1.00 | 13.78 | 6 | 4369 | CG | LVS A 561 | 1.847 | 66.177 | 52.656 | 1.00 | 22.42 | 6 |
| 4328 | O | ALA A 555 | 1.051 | 78.305 | 39.204 | 1.00 | 14.85 | 8 | 4370 | CD | LVS A 561 | 1.025 | 67.110 | 53.523 | 1.00 | 25.69 | 6 |
| 4329 | CB | ALA A 555 | 1.375 | 77.200 | 36.142 | 1.00 | 16.26 | 6 | 4371 | CE | LVS A 561 | -0.461 | 66.912 | 53.312 | 1.00 | 33.13 | 6 |
| 4330 | N | GLY A 556 | 2.874 | 76.966 | 38.857 | 1.00 | 12.02 | 7 | 4372 | NZ | LVS A 561 | -1.198 | 68.004 | 54.033 | 1.00 | 37.04 | 7 |
| 4331 | CA | GLY A 556 | 3.602 | 77.675 | 39.947 | 1.00 | 14.17 | 6 | 4373 | N | VAL A 562 | 2.947 | 63.489 | 51.047 | 1.00 | 16.07 | 7 |
| 4332 | C | GLY A 556 | 4.312 | 76.639 | 40.815 | 1.00 | 12.79 | 6 | 4374 | CA | VAL A 562 | 2.525 | 62.108 | 51.051 | 1.00 | 14.01 | 6 |
| 4333 | O | GLY A 556 | 4.121 | 75.415 | 40.670 | 1.00 | 12.92 | 8 | 4375 | C | VAL A 562 | 1.751 | 61.827 | 52.382 | 1.00 | 14.81 | 6 |
| 4334 | N | LEU A 557 | 5.203 | 77.130 | 41.670 | 1.00 | 13.81 | 7 | 4376 | O | VAL A 562 | 2.150 | 62.324 | 53.398 | 1.00 | 17.73 | 8 |
| 4335 | CA | LEU A 557 | 5.876 | 76.232 | 42.626 | 1.00 | 13.54 | 6 | 4377 | CB | VAL A 562 | 3.735 | 61.158 | 51.036 | 1.00 | 16.60 | 6 |
| 4336 | C | LEU A 557 | 4.918 | 75.806 | 43.737 | 1.00 | 12.41 | 6 | 4378 | CG1 | VAL A 562 | 3.312 | 59.677 | 51.185 | 1.00 | 16.48 | 6 |
| 4337 | O | LEU A 557 | 4.110 | 76.659 | 44.188 | 1.00 | 14.95 | 8 | 4379 | CG2 | VAL A 562 | 4.473 | 61.228 | 49.672 | 1.00 | 17.80 | 6 |
| 4338 | CB | LEU A 557 | 7.091 | 76.999 | 43.221 | 1.00 | 13.41 | 6 | 4380 | N | THR A 563 | 0.603 | 61.156 | 52.140 | 1.00 | 17.67 | 7 |
| 4339 | CG | LEU A 557 | 8.018 | 76.123 | 44.069 | 1.00 | 15.11 | 6 | 4381 | CA | THR A 563 | -0.181 | 60.806 | 53.380 | 1.00 | 18.18 | 6 |
| 4340 | CD1 | LEU A 557 | 8.847 | 75.220 | 43.141 | 1.00 | 13.33 | 6 | 4382 | C | THR A 563 | -0.261 | 59.308 | 53.412 | 1.00 | 18.30 | 6 |
| 4341 | CD2 | LEU A 557 | 8.965 | 77.046 | 44.898 | 1.00 | 17.39 | 6 | 4383 | O | THR A 563 | -0.679 | 58.642 | 52.456 | 1.00 | 19.93 | 8 |
| 4342 | N | THR A 558 | 4.801 | 74.500 | 43.858 | 1.00 | 13.24 | 7 | 4384 | CB | THR A 563 | -1.542 | 61.496 | 53.361 | 1.00 | 18.11 | 6 |
| 4343 | CA | THR A 558 | 3.807 | 73.941 | 44.818 | 1.00 | 13.26 | 6 | 4385 | OG1 | THR A 563 | -1.367 | 62.891 | 53.406 | 1.00 | 19.44 | 8 |

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|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|------|-----|------|---|-----|--------|--------|--------|------|-------|---|
| 4386 | CG2 | THR | A | 563 | -2.281 | 61.112 | 54.705 | 1.00 | 20.36 | 6 | 4428 | CA | LEU | A | 571 | 6.705 | 68.878 | 52.131 | 1.00 | 12.49 | 6 |
| 4387 | N | ALA | A | 564 | 0.154 | 58.701 | 54.548 | 1.00 | 21.05 | 7 | 4429 | C | LEU | A | 571 | 7.959 | 69.019 | 51.282 | 1.00 | 15.87 | 6 |
| 4388 | CA | ALA | A | 564 | 0.245 | 57.258 | 54.649 | 1.00 | 24.26 | 6 | 4430 | O | LEU | A | 571 | 9.024 | 69.355 | 51.828 | 1.00 | 16.79 | 8 |
| 4389 | C | ALA | A | 564 | -0.234 | 56.845 | 56.060 | 1.00 | 23.28 | 6 | 4431 | CB | LEU | A | 571 | 6.147 | 70.286 | 52.340 | 1.00 | 15.18 | 6 |
| 4390 | O | ALA | A | 564 | 0.104 | 57.536 | 57.008 | 1.00 | 21.58 | 8 | 4432 | CB | LEU | A | 571 | 4.911 | 70.396 | 53.250 | 1.00 | 22.77 | 6 |
| 4391 | CB | ALA | A | 564 | 1.658 | 56.711 | 54.437 | 1.00 | 25.03 | 6 | 4433 | CD1 | LEU | A | 571 | 4.368 | 71.807 | 53.300 | 1.00 | 22.26 | 6 |
| 4392 | N | GLY | A | 565 | -1.218 | 55.968 | 56.140 | 1.00 | 30.08 | 7 | 4434 | CD2 | LEU | A | 571 | 3.834 | 69.448 | 52.757 | 1.00 | 22.04 | 6 |
| 4393 | CA | GLY | A | 565 | -1.857 | 55.701 | 57.443 | 1.00 | 31.09 | 6 | 4435 | N | TYR | A | 572 | 7.747 | 68.878 | 49.946 | 1.00 | 13.65 | 7 |
| 4394 | C | GLY | A | 565 | -2.488 | 56.887 | 58.121 | 1.00 | 35.06 | 6 | 4436 | CA | TYR | A | 572 | 8.930 | 69.100 | 49.067 | 1.00 | 12.87 | 6 |
| 4395 | O | GLY | A | 565 | -2.493 | 56.983 | 59.363 | 1.00 | 31.36 | 8 | 4437 | C | TYR | A | 572 | 8.322 | 69.878 | 47.880 | 1.00 | 14.52 | 6 |
| 4396 | N | GLY | A | 566 | -3.025 | 57.873 | 57.403 | 1.00 | 32.22 | 7 | 4438 | O | TYR | A | 572 | 7.347 | 69.399 | 47.262 | 1.00 | 14.71 | 8 |
| 4397 | CA | GLY | A | 566 | -3.549 | 59.083 | 58.011 | 1.00 | 31.70 | 6 | 4439 | CB | TYR | A | 572 | 9.480 | 67.704 | 48.701 | 1.00 | 12.62 | 6 |
| 4398 | C | GLY | A | 566 | -2.523 | 60.107 | 58.438 | 1.00 | 31.07 | 6 | 4440 | CG | TYR | A | 572 | 10.887 | 67.679 | 48.121 | 1.00 | 13.61 | 6 |
| 4399 | O | GLY | A | 566 | -2.936 | 61.213 | 58.829 | 1.00 | 32.69 | 8 | 4441 | CD1 | TYR | A | 572 | 11.079 | 68.175 | 46.835 | 1.00 | 13.57 | 6 |
| 4400 | N | VAL | A | 567 | -1.202 | 59.887 | 58.271 | 1.00 | 26.17 | 7 | 4442 | CD2 | TYR | A | 572 | 11.946 | 67.161 | 48.845 | 1.00 | 15.40 | 6 |
| 4401 | CA | VAL | A | 567 | -0.186 | 60.798 | 58.776 | 1.00 | 21.45 | 6 | 4443 | CE1 | TYR | A | 572 | 12.361 | 68.168 | 46.257 | 1.00 | 13.80 | 6 |
| 4402 | C | VAL | A | 567 | 0.537 | 61.488 | 57.557 | 1.00 | 17.95 | 6 | 4444 | CE2 | TYR | A | 572 | 13.221 | 67.135 | 48.283 | 1.00 | 12.70 | 6 |
| 4403 | O | VAL | A | 567 | 0.692 | 60.707 | 56.658 | 1.00 | 18.75 | 8 | 4445 | CZ | TYR | A | 572 | 13.400 | 67.529 | 47.002 | 1.00 | 14.33 | 6 |
| 4404 | CB | VAL | A | 567 | 0.945 | 60.023 | 59.500 | 1.00 | 26.89 | 6 | 4446 | OH | TYR | A | 572 | 14.710 | 67.607 | 46.466 | 1.00 | 13.40 | 8 |
| 4405 | CG1 | VAL | A | 567 | 1.981 | 60.946 | 60.096 | 1.00 | 30.00 | 6 | 4447 | N | SER | A | 573 | 9.060 | 70.874 | 47.387 | 1.00 | 13.37 | 7 |
| 4406 | CG2 | VAL | A | 567 | 0.308 | 59.088 | 60.567 | 1.00 | 33.86 | 6 | 4448 | CA | SER | A | 573 | 8.571 | 71.734 | 46.294 | 1.00 | 12.21 | 6 |
| 4407 | N | SER | A | 568 | 0.687 | 62.774 | 57.699 | 1.00 | 19.77 | 7 | 4449 | C | SER | A | 573 | 8.665 | 71.055 | 44.920 | 1.00 | 12.75 | 6 |
| 4408 | CA | SER | A | 568 | 1.267 | 63.410 | 56.486 | 1.00 | 19.16 | 6 | 4450 | O | SER | A | 573 | 9.520 | 70.234 | 44.703 | 1.00 | 12.64 | 8 |
| 4409 | C | SER | A | 568 | 2.770 | 63.585 | 56.688 | 1.00 | 19.28 | 6 | 4451 | CB | ASER | A | 573 | 9.436 | 72.999 | 46.162 | 0.60 | 17.33 | 6 |
| 4410 | O | SER | A | 568 | 3.351 | 63.752 | 57.763 | 1.00 | 21.35 | 8 | 4452 | OG | ASER | A | 573 | 9.459 | 73.767 | 47.331 | 0.60 | 22.77 | 8 |
| 4411 | CB | SER | A | 568 | 0.574 | 64.705 | 56.156 | 1.00 | 29.69 | 6 | 4452 | CB | BSER | A | 573 | 9.408 | 73.025 | 46.276 | 0.40 | 15.40 | 6 |
| 4412 | OG | SER | A | 568 | 0.595 | 65.549 | 57.266 | 1.00 | 41.18 | 8 | 4453 | OG | BSER | A | 573 | 10.793 | 72.728 | 46.149 | 0.40 | 16.17 | 8 |
| 4413 | N | SER | A | 569 | 3.399 | 63.581 | 55.503 | 1.00 | 19.22 | 7 | 4453 | N | TYR | A | 574 | 7.838 | 71.568 | 44.000 | 1.00 | 11.56 | 7 |
| 4414 | CA | SER | A | 569 | 4.867 | 63.784 | 55.480 | 1.00 | 17.43 | 6 | 4454 | CA | TYR | A | 574 | 7.912 | 71.077 | 42.604 | 1.00 | 10.89 | 6 |
| 4415 | C | SER | A | 569 | 5.229 | 65.245 | 55.568 | 1.00 | 17.17 | 6 | 4455 | C | TYR | A | 574 | 7.374 | 72.249 | 42.138 | 1.00 | 13.28 | 6 |
| 4416 | O | SER | A | 569 | 4.519 | 66.266 | 55.502 | 1.00 | 17.53 | 8 | 4456 | O | TYR | A | 574 | 6.344 | 72.860 | 42.138 | 1.00 | 12.17 | 8 |
| 4417 | CB | SER | A | 569 | 5.381 | 63.220 | 54.137 | 1.00 | 17.58 | 6 | 4457 | CB | TYR | A | 574 | 7.041 | 69.857 | 42.405 | 1.00 | 11.94 | 6 |
| 4418 | OG | SER | A | 569 | 5.066 | 64.083 | 53.025 | 1.00 | 15.50 | 8 | 4458 | CG | TYR | A | 574 | 6.917 | 69.379 | 40.971 | 1.00 | 11.37 | 6 |
| 4419 | N | ASN | A | 570 | 6.572 | 65.473 | 55.538 | 1.00 | 14.77 | 7 | 4459 | CD1 | TYR | A | 574 | 7.921 | 68.521 | 40.467 | 1.00 | 12.69 | 6 |
| 4420 | CA | ASN | A | 570 | 7.143 | 66.776 | 55.253 | 1.00 | 13.84 | 6 | 4460 | CD2 | TYR | A | 574 | 5.867 | 69.781 | 40.162 | 1.00 | 11.85 | 6 |
| 4421 | C | ASN | A | 570 | 6.848 | 67.107 | 53.752 | 1.00 | 13.33 | 6 | 4461 | CE1 | TYR | A | 574 | 7.863 | 68.052 | 39.154 | 1.00 | 13.23 | 6 |
| 4422 | O | ASN | A | 570 | 6.527 | 66.217 | 52.996 | 1.00 | 16.50 | 8 | 4462 | CE2 | TYR | A | 574 | 5.792 | 69.313 | 38.834 | 1.00 | 13.93 | 6 |
| 4423 | CB | ASN | A | 570 | 8.670 | 66.723 | 55.435 | 1.00 | 17.22 | 6 | 4463 | CZ | TYR | A | 574 | 6.796 | 68.466 | 38.366 | 1.00 | 11.32 | 6 |
| 4424 | CG | ASN | A | 570 | 9.363 | 65.581 | 54.758 | 1.00 | 16.95 | 6 | 4464 | OH | TYR | A | 574 | 6.679 | 68.006 | 37.078 | 1.00 | 12.54 | 8 |
| 4425 | OD1 | ASN | A | 570 | 9.038 | 64.399 | 54.745 | 1.00 | 15.12 | 8 | 4465 | N | ASN | A | 575 | 7.992 | 72.510 | 40.627 | 1.00 | 12.18 | 7 |
| 4426 | ND2 | ASN | A | 570 | 10.455 | 65.853 | 54.023 | 1.00 | 16.51 | 7 | 4466 | CA | ASN | A | 575 | 7.578 | 73.682 | 39.820 | 1.00 | 12.18 | 6 |
| 4427 | N | LEU | A | 571 | 7.108 | 68.381 | 53.486 | 1.00 | 14.82 | 7 | 4467 | C | ASN | A | 575 | 6.738 | 73.306 | 38.608 | 1.00 | 12.59 | 6 |

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|------|-----|-----------|-------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4468 | O | ASN A 575 | 7.171 | 72.699 | 37.598 | 1.00 | 12.20 | 8 | 4510 | CB | GLN A 581 | 8.751 | 75.601 | 27.465 | 1.00 | 11.27 | 6 |
| 4469 | O | ASN A 575 | 8.898 | 74.351 | 39.331 | 1.00 | 12.02 | 6 | 4511 | CG | GLN A 581 | 8.407 | 75.301 | 28.975 | 1.00 | 10.49 | 6 |
| 4470 | CG | ASN A 575 | 8.635 | 75.707 | 38.700 | 1.00 | 17.00 | 6 | 4512 | CD | GLN A 581 | 7.920 | 76.579 | 29.654 | 1.00 | 12.45 | 6 |
| 4471 | OD1 | ASN A 575 | 7.562 | 76.292 | 38.872 | 1.00 | 14.54 | 8 | 4513 | OE1 | GLN A 581 | 8.545 | 77.588 | 29.921 | 1.00 | 13.44 | 8 |
| 4472 | ND2 | ASN A 575 | 9.608 | 76.223 | 37.934 | 1.00 | 13.02 | 7 | 4514 | NE2 | GLN A 581 | 6.582 | 76.528 | 30.002 | 1.00 | 11.11 | 7 |
| 4473 | N | ILE A 576 | 5.400 | 73.515 | 38.739 | 1.00 | 10.95 | 7 | 4515 | N | THR A 582 | 8.202 | 77.209 | 24.953 | 1.00 | 9.52 | 7 |
| 4474 | CA | ILE A 576 | 4.506 | 73.221 | 37.604 | 1.00 | 10.36 | 6 | 4516 | CA | THR A 582 | 8.978 | 77.646 | 23.772 | 1.00 | 10.13 | 6 |
| 4475 | C | ILE A 576 | 4.485 | 74.374 | 36.602 | 1.00 | 12.05 | 6 | 4517 | C | THR A 582 | 10.049 | 78.609 | 24.293 | 1.00 | 10.70 | 6 |
| 4476 | O | ILE A 576 | 4.145 | 75.497 | 36.930 | 1.00 | 13.39 | 8 | 4518 | O | THR A 582 | 9.921 | 79.235 | 25.313 | 1.00 | 12.73 | 8 |
| 4477 | CB | ILE A 576 | 3.036 | 73.061 | 38.127 | 1.00 | 12.95 | 6 | 4519 | CB | THR A 582 | 8.018 | 78.306 | 22.763 | 1.00 | 12.88 | 6 |
| 4478 | CG1 | ILE A 576 | 3.082 | 71.956 | 39.190 | 1.00 | 13.10 | 6 | 4520 | OG1 | THR A 582 | 8.736 | 78.798 | 21.599 | 1.00 | 12.92 | 8 |
| 4479 | CG2 | ILE A 576 | 2.079 | 72.677 | 36.966 | 1.00 | 14.18 | 6 | 4521 | CG2 | THR A 582 | 7.265 | 79.504 | 23.359 | 1.00 | 11.55 | 6 |
| 4480 | CD1 | ILE A 576 | 1.709 | 71.488 | 39.691 | 1.00 | 15.07 | 6 | 4522 | N | SER A 583 | 11.166 | 78.712 | 23.507 | 1.00 | 11.67 | 7 |
| 4481 | N | LEU A 577 | 4.883 | 74.054 | 35.368 | 1.00 | 10.51 | 7 | 4523 | CA | SER A 583 | 12.321 | 79.527 | 23.931 | 1.00 | 12.58 | 6 |
| 4482 | CA | LEU A 577 | 4.908 | 75.052 | 34.303 | 1.00 | 12.74 | 6 | 4524 | C | SER A 583 | 12.300 | 80.783 | 23.061 | 1.00 | 11.58 | 6 |
| 4483 | C | LEU A 577 | 3.480 | 75.308 | 33.772 | 1.00 | 11.80 | 6 | 4525 | O | SER A 583 | 12.496 | 80.687 | 21.844 | 1.00 | 12.44 | 8 |
| 4484 | O | LEU A 577 | 2.572 | 74.474 | 34.021 | 1.00 | 13.37 | 8 | 4526 | CB | SER A 583 | 13.612 | 78.697 | 23.747 | 1.00 | 12.53 | 6 |
| 4485 | CB | LEU A 577 | 5.757 | 74.463 | 33.137 | 1.00 | 11.48 | 6 | 4527 | OG | SER A 583 | 14.755 | 79.449 | 24.240 | 1.00 | 14.73 | 8 |
| 4486 | CG | LEU A 577 | 7.226 | 74.238 | 33.569 | 1.00 | 12.21 | 6 | 4528 | N | VAL A 584 | 12.118 | 81.899 | 23.781 | 1.00 | 10.19 | 7 |
| 4487 | CD1 | LEU A 577 | 7.982 | 73.601 | 32.421 | 1.00 | 13.03 | 6 | 4529 | CA | VAL A 584 | 11.741 | 83.141 | 23.016 | 1.00 | 9.76 | 6 |
| 4488 | CD2 | LEU A 577 | 7.897 | 75.576 | 33.989 | 1.00 | 13.85 | 6 | 4530 | C | VAL A 584 | 12.721 | 84.268 | 23.298 | 1.00 | 11.27 | 6 |
| 4489 | N | SER A 578 | 3.398 | 76.385 | 33.006 | 1.00 | 11.76 | 7 | 4531 | O | VAL A 584 | 13.066 | 84.570 | 24.440 | 1.00 | 11.87 | 8 |
| 4490 | CA | SER A 578 | 2.037 | 76.726 | 32.475 | 1.00 | 15.00 | 6 | 4532 | CB | VAL A 584 | 10.358 | 83.645 | 23.506 | 1.00 | 12.33 | 6 |
| 4491 | C | SER A 578 | 1.681 | 75.960 | 31.215 | 1.00 | 17.37 | 6 | 4533 | CG1 | VAL A 584 | 10.041 | 84.968 | 22.757 | 1.00 | 14.53 | 6 |
| 4492 | O | SER A 578 | 0.553 | 76.134 | 30.685 | 1.00 | 17.93 | 8 | 4534 | CG2 | VAL A 584 | 9.279 | 82.604 | 23.220 | 1.00 | 12.71 | 6 |
| 4493 | CB | SER A 578 | 2.081 | 78.230 | 32.132 | 1.00 | 13.25 | 6 | 4535 | N | VAL A 585 | 13.307 | 84.868 | 22.244 | 1.00 | 10.77 | 7 |
| 4494 | OG | SER A 578 | 2.321 | 78.967 | 33.305 | 1.00 | 14.45 | 8 | 4536 | CA | VAL A 585 | 14.166 | 86.030 | 22.421 | 1.00 | 9.69 | 6 |
| 4495 | N | GLY A 579 | 2.538 | 75.095 | 30.688 | 1.00 | 15.28 | 7 | 4537 | C | VAL A 585 | 13.244 | 87.219 | 22.693 | 1.00 | 12.06 | 6 |
| 4496 | CA | GLY A 579 | 2.266 | 74.270 | 29.497 | 1.00 | 14.88 | 6 | 4538 | O | VAL A 585 | 12.450 | 87.576 | 21.803 | 1.00 | 14.60 | 8 |
| 4497 | C | GLY A 579 | 3.627 | 74.010 | 28.818 | 1.00 | 13.39 | 6 | 4539 | CB | VAL A 585 | 14.882 | 86.310 | 21.064 | 1.00 | 11.53 | 6 |
| 4498 | O | GLY A 579 | 4.670 | 74.450 | 29.318 | 1.00 | 14.78 | 8 | 4540 | CG1 | VAL A 585 | 15.712 | 87.605 | 21.158 | 1.00 | 15.03 | 6 |
| 4499 | N | THR A 580 | 3.518 | 73.227 | 27.740 | 1.00 | 11.35 | 7 | 4541 | CG2 | VAL A 585 | 15.750 | 85.111 | 20.717 | 1.00 | 14.67 | 6 |
| 4500 | CA | THR A 580 | 4.803 | 72.961 | 27.005 | 1.00 | 13.16 | 6 | 4542 | N | PHE A 586 | 13.361 | 87.762 | 23.908 | 1.00 | 12.32 | 7 |
| 4501 | C | THR A 580 | 5.419 | 74.292 | 26.647 | 1.00 | 14.61 | 6 | 4543 | CA | PHE A 586 | 12.622 | 88.986 | 24.243 | 1.00 | 12.19 | 6 |
| 4502 | O | THR A 580 | 4.747 | 75.282 | 26.349 | 1.00 | 14.26 | 8 | 4544 | C | PHE A 586 | 13.584 | 90.161 | 24.063 | 1.00 | 14.77 | 6 |
| 4503 | CB | THR A 580 | 4.517 | 72.009 | 25.835 | 1.00 | 13.57 | 6 | 4545 | O | PHE A 586 | 14.668 | 90.209 | 24.709 | 1.00 | 12.38 | 8 |
| 4504 | OG1 | THR A 580 | 5.753 | 71.676 | 25.176 | 1.00 | 16.06 | 8 | 4546 | CB | PHE A 586 | 12.174 | 88.944 | 25.704 | 1.00 | 12.57 | 6 |
| 4505 | CG2 | THR A 580 | 3.688 | 72.715 | 24.732 | 1.00 | 20.75 | 6 | 4547 | CG | PHE A 586 | 10.886 | 88.184 | 25.987 | 1.00 | 11.39 | 6 |
| 4506 | N | GLN A 581 | 6.787 | 74.346 | 26.706 | 1.00 | 11.89 | 7 | 4548 | CD1 | PHE A 586 | 10.879 | 86.809 | 26.009 | 1.00 | 13.56 | 6 |
| 4507 | CA | GLN A 581 | 7.454 | 75.658 | 26.609 | 1.00 | 10.06 | 6 | 4549 | CD2 | PHE A 586 | 9.694 | 88.868 | 26.231 | 1.00 | 13.70 | 6 |
| 4508 | C | GLN A 581 | 8.012 | 75.905 | 25.148 | 1.00 | 10.19 | 6 | 4550 | CE1 | PHE A 586 | 9.758 | 86.060 | 26.284 | 1.00 | 13.86 | 6 |
| 4509 | O | GLN A 581 | 8.163 | 75.020 | 24.338 | 1.00 | 12.94 | 8 | 4551 | CE2 | PHE A 586 | 8.543 | 88.102 | 26.520 | 1.00 | 12.32 | 6 |

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|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 4552 | CZ | PHE A 586 | 8.577 | 86.707 | 26.558 | 1.00 | 11.70 | 6 | 4594 | N | PRO A 593 | 18.778 | 105.367 | 29.550 | 1.00 | 21.02 | 7 |
| 4553 | N | THR A 587 | 13.189 | 91.146 | 23.239 | 1.00 | 14.16 | 7 | 4595 | CA | PRO A 593 | 20.204 | 105.252 | 29.779 | 1.00 | 20.83 | 6 |
| 4554 | CA | THR A 587 | 14.016 | 92.324 | 23.066 | 1.00 | 12.96 | 6 | 4596 | C | PRO A 593 | 20.494 | 104.537 | 31.094 | 1.00 | 20.17 | 6 |
| 4555 | C | THR A 587 | 13.247 | 93.561 | 23.468 | 1.00 | 13.58 | 6 | 4597 | O | PRO A 593 | 19.811 | 104.784 | 32.102 | 1.00 | 21.50 | 8 |
| 4556 | O | THR A 587 | 12.072 | 93.651 | 23.058 | 1.00 | 15.22 | 8 | 4598 | CB | PRO A 593 | 20.715 | 106.727 | 29.941 | 1.00 | 22.70 | 6 |
| 4557 | CB | THR A 587 | 14.421 | 92.464 | 21.555 | 1.00 | 11.66 | 6 | 4599 | CG | PRO A 593 | 19.643 | 107.491 | 29.165 | 1.00 | 24.71 | 6 |
| 4558 | OG1 | THR A 587 | 15.145 | 91.299 | 21.141 | 1.00 | 15.06 | 8 | 4600 | CD | PRO A 593 | 18.337 | 106.774 | 29.432 | 1.00 | 23.44 | 6 |
| 4559 | CG2 | THR A 587 | 15.331 | 93.708 | 21.318 | 1.00 | 13.37 | 6 | 4601 | N | THR A 594 | 21.530 | 103.723 | 31.165 | 1.00 | 19.91 | 7 |
| 4560 | N | VAL A 588 | 13.829 | 94.487 | 24.195 | 1.00 | 14.03 | 7 | 4602 | CA | THR A 594 | 21.909 | 103.060 | 32.402 | 1.00 | 21.78 | 6 |
| 4561 | CA | VAL A 588 | 13.156 | 95.779 | 24.469 | 1.00 | 14.79 | 6 | 4603 | C | THR A 594 | 23.380 | 103.366 | 32.686 | 1.00 | 23.13 | 6 |
| 4562 | C | VAL A 588 | 14.079 | 96.867 | 23.912 | 1.00 | 14.40 | 6 | 4604 | O | THR A 594 | 24.138 | 103.737 | 31.787 | 1.00 | 23.96 | 8 |
| 4563 | O | VAL A 588 | 15.258 | 97.015 | 24.225 | 1.00 | 15.56 | 8 | 4605 | CB | THR A 594 | 21.729 | 101.521 | 32.292 | 1.00 | 23.27 | 6 |
| 4564 | CB | VAL A 588 | 12.863 | 95.933 | 25.971 | 1.00 | 14.24 | 6 | 4606 | OG1 | THR A 594 | 22.466 | 101.094 | 31.140 | 1.00 | 20.06 | 8 |
| 4565 | CG1 | VAL A 588 | 14.111 | 95.935 | 26.870 | 1.00 | 14.60 | 6 | 4607 | CG2 | THR A 594 | 20.245 | 101.183 | 32.157 | 1.00 | 21.33 | 6 |
| 4566 | CG2 | VAL A 588 | 12.079 | 97.255 | 26.232 | 1.00 | 13.38 | 6 | 4608 | N | ASN A 595 | 23.764 | 103.210 | 33.928 | 1.00 | 23.96 | 7 |
| 4567 | N | LYS A 589 | 13.478 | 97.570 | 22.915 | 1.00 | 15.39 | 7 | 4609 | CA | ASN A 595 | 25.142 | 103.193 | 34.370 | 1.00 | 28.93 | 6 |
| 4568 | CA | LYS A 589 | 14.212 | 98.670 | 22.258 | 1.00 | 16.20 | 6 | 4610 | C | ASN A 595 | 25.614 | 101.791 | 34.716 | 1.00 | 31.88 | 6 |
| 4569 | C | LYS A 589 | 14.180 | 100.009 | 22.953 | 1.00 | 18.01 | 6 | 4611 | O | ASN A 595 | 24.847 | 100.849 | 34.915 | 1.00 | 22.74 | 8 |
| 4570 | O | LYS A 589 | 13.230 | 100.355 | 23.652 | 1.00 | 15.39 | 8 | 4612 | CB | ASN A 595 | 25.285 | 104.099 | 35.620 | 1.00 | 34.82 | 6 |
| 4571 | CB | LYS A 589 | 13.597 | 98.820 | 20.860 | 1.00 | 16.23 | 6 | 4613 | CG | ASN A 595 | 24.970 | 105.532 | 35.180 | 1.00 | 36.76 | 6 |
| 4572 | CG | LYS A 589 | 13.908 | 97.588 | 20.008 | 1.00 | 17.01 | 6 | 4614 | OD1 | ASN A 595 | 24.047 | 106.190 | 35.647 | 1.00 | 42.57 | 8 |
| 4573 | CD | LYS A 589 | 13.275 | 97.825 | 18.634 | 1.00 | 24.71 | 6 | 4615 | ND2 | ASN A 595 | 25.738 | 106.004 | 34.208 | 1.00 | 38.16 | 7 |
| 4574 | CE | LYS A 589 | 13.494 | 96.582 | 17.792 | 1.00 | 37.49 | 6 | 4616 | N | LEU A 596 | 26.939 | 101.654 | 34.839 | 1.00 | 34.83 | 7 |
| 4575 | NZ | LYS A 589 | 13.368 | 96.852 | 16.321 | 1.00 | 51.36 | 7 | 4617 | CA | LEU A 596 | 27.559 | 100.380 | 35.212 | 1.00 | 37.55 | 6 |
| 4576 | N | SER A 590 | 15.302 | 100.747 | 22.828 | 1.00 | 16.34 | 7 | 4618 | C | LEU A 596 | 26.947 | 99.803 | 36.488 | 1.00 | 31.76 | 6 |
| 4577 | CA | SER A 590 | 15.371 | 102.116 | 23.293 | 1.00 | 19.32 | 6 | 4619 | O | LEU A 596 | 26.589 | 100.502 | 37.435 | 1.00 | 35.49 | 8 |
| 4578 | C | SER A 590 | 15.006 | 102.295 | 24.746 | 1.00 | 19.68 | 6 | 4620 | CB | LEU A 596 | 29.051 | 100.642 | 35.407 | 1.00 | 48.79 | 6 |
| 4579 | O | SER A 590 | 14.185 | 103.146 | 25.151 | 1.00 | 17.24 | 8 | 4621 | CG | LEU A 596 | 30.042 | 99.528 | 35.681 | 1.00 | 52.60 | 6 |
| 4580 | CB | SER A 590 | 14.448 | 103.009 | 22.421 | 1.00 | 20.32 | 6 | 4622 | CD1 | LEU A 596 | 29.894 | 98.971 | 37.092 | 1.00 | 56.16 | 6 |
| 4581 | OG | SER A 590 | 14.867 | 102.933 | 21.046 | 1.00 | 22.81 | 8 | 4623 | CD2 | LEU A 596 | 29.934 | 98.433 | 34.628 | 1.00 | 56.63 | 6 |
| 4582 | N | ALA A 591 | 15.698 | 101.514 | 25.612 | 1.00 | 17.08 | 7 | 4624 | N | GLY A 597 | 26.492 | 98.556 | 36.348 | 1.00 | 30.34 | 7 |
| 4583 | CA | ALA A 591 | 15.458 | 101.617 | 27.048 | 1.00 | 16.02 | 6 | 4625 | CA | GLY A 597 | 25.861 | 97.860 | 37.473 | 1.00 | 30.50 | 6 |
| 4584 | C | ALA A 591 | 16.178 | 102.871 | 27.530 | 1.00 | 18.06 | 6 | 4626 | C | GLY A 597 | 24.337 | 97.822 | 37.288 | 1.00 | 25.20 | 6 |
| 4585 | O | ALA A 591 | 17.152 | 103.325 | 26.878 | 1.00 | 15.85 | 8 | 4627 | O | GLY A 597 | 23.705 | 96.996 | 37.949 | 1.00 | 23.57 | 8 |
| 4586 | CB | ALA A 591 | 16.045 | 100.326 | 27.695 | 1.00 | 15.17 | 6 | 4628 | N | ASP A 598 | 23.780 | 98.803 | 36.544 | 1.00 | 21.92 | 7 |
| 4587 | N | PRO A 592 | 15.872 | 103.303 | 28.730 | 1.00 | 18.28 | 7 | 4629 | CA | ASP A 598 | 22.315 | 98.799 | 36.399 | 1.00 | 18.64 | 6 |
| 4588 | CA | PRO A 592 | 16.493 | 104.529 | 29.298 | 1.00 | 18.18 | 6 | 4630 | C | ASP A 598 | 21.982 | 97.666 | 35.429 | 1.00 | 21.53 | 6 |
| 4589 | C | PRO A 592 | 17.967 | 104.319 | 29.512 | 1.00 | 22.69 | 6 | 4631 | O | ASP A 598 | 22.702 | 97.563 | 34.399 | 1.00 | 20.69 | 8 |
| 4590 | O | PRO A 592 | 18.463 | 103.180 | 29.693 | 1.00 | 19.12 | 8 | 4632 | CB | ASP A 598 | 21.814 | 100.096 | 35.763 | 1.00 | 17.61 | 6 |
| 4591 | CB | PRO A 592 | 15.762 | 104.797 | 30.621 | 1.00 | 19.23 | 6 | 4633 | CG | ASP A 598 | 22.046 | 101.382 | 36.536 | 1.00 | 20.17 | 6 |
| 4592 | CG | PRO A 592 | 14.433 | 104.085 | 30.387 | 1.00 | 23.18 | 6 | 4634 | OD1 | ASP A 598 | 22.364 | 101.347 | 37.751 | 1.00 | 19.25 | 8 |
| 4593 | CD | PRO A 592 | 14.795 | 102.833 | 29.585 | 1.00 | 17.71 | 6 | 4635 | OD2 | ASP A 598 | 21.858 | 102.432 | 35.868 | 1.00 | 22.20 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 4636 | N | LYS A 599 | 20.861 | 96.919 | 35.612 | 1.00 | 18.66 | 7 | 4678 | OG1 THR A 603 | 7.971 | 90.241 | 36.987 | 1.00 | 14.53 | 8 |
| 4637 | CA | LYS A 599 | 20.593 | 95.891 | 34.605 | 1.00 | 15.76 | 6 | 4679 | CG2 THR A 603 | 8.152 | 92.414 | 35.971 | 1.00 | 15.35 | 6 |
| 4638 | C | LYS A 599 | 19.056 | 95.824 | 34.461 | 1.00 | 11.90 | 6 | 4680 | N GLY A 604 | 6.310 | 89.331 | 34.489 | 1.00 | 11.51 | 7 |
| 4639 | O | LYS A 599 | 18.320 | 96.237 | 35.358 | 1.00 | 19.04 | 8 | 4681 | CA GLY A 604 | 4.995 | 89.274 | 33.787 | 1.00 | 11.82 | 6 |
| 4640 | CB | LYS A 599 | 21.049 | 94.484 | 35.006 | 1.00 | 23.86 | 6 | 4682 | C GLY A 604 | 4.042 | 88.348 | 34.530 | 1.00 | 12.03 | 6 |
| 4641 | CG | LYS A 599 | 22.597 | 94.419 | 35.031 | 1.00 | 25.32 | 6 | 4683 | O GLY A 604 | 4.358 | 87.909 | 35.636 | 1.00 | 13.68 | 8 |
| 4642 | CD | LYS A 599 | 23.118 | 93.007 | 35.252 | 1.00 | 26.43 | 6 | 4684 | N ASN A 605 | 2.911 | 88.082 | 33.859 | 1.00 | 12.03 | 7 |
| 4643 | CE | LYS A 599 | 24.656 | 93.063 | 35.120 | 1.00 | 32.43 | 6 | 4685 | CA ASN A 605 | 1.782 | 87.516 | 34.637 | 1.00 | 11.85 | 6 |
| 4644 | NZ | LYS A 599 | 25.179 | 91.656 | 35.106 | 1.00 | 35.89 | 7 | 4686 | C ASN A 605 | 1.680 | 86.017 | 34.575 | 1.00 | 12.50 | 6 |
| 4645 | N | ILE A 600 | 18.623 | 95.442 | 33.287 | 1.00 | 13.51 | 7 | 4687 | O ASN A 605 | 0.615 | 85.441 | 34.625 | 1.00 | 14.07 | 8 |
| 4646 | CA | ILE A 600 | 17.178 | 95.336 | 33.021 | 1.00 | 12.20 | 6 | 4688 | CB ASN A 605 | 0.481 | 88.161 | 34.031 | 1.00 | 13.77 | 6 |
| 4647 | C | ILE A 600 | 16.746 | 93.886 | 33.130 | 1.00 | 13.74 | 6 | 4689 | CG ASN A 605 | 0.265 | 87.610 | 32.629 | 1.00 | 17.19 | 6 |
| 4648 | O | ILE A 600 | 17.476 | 92.927 | 32.799 | 1.00 | 14.24 | 8 | 4690 | OD1 ASN A 605 | 1.080 | 87.101 | 31.828 | 1.00 | 13.63 | 8 |
| 4649 | CB | ILE A 600 | 16.938 | 95.829 | 31.554 | 1.00 | 13.87 | 6 | 4691 | ND2 ASN A 605 | -1.025 | 87.681 | 32.165 | 1.00 | 16.36 | 7 |
| 4650 | CG1 | ILE A 600 | 17.249 | 97.335 | 31.566 | 1.00 | 21.52 | 6 | 4692 | N ILE A 606 | 2.823 | 85.308 | 34.560 | 1.00 | 13.26 | 7 |
| 4651 | CG2 | ILE A 600 | 15.499 | 95.618 | 31.051 | 1.00 | 15.85 | 6 | 4693 | CA ILE A 606 | 2.836 | 83.860 | 34.628 | 1.00 | 11.73 | 6 |
| 4652 | CD1 | ILE A 600 | 16.798 | 98.104 | 30.313 | 1.00 | 23.52 | 6 | 4694 | C ILE A 606 | 4.099 | 83.493 | 35.448 | 1.00 | 13.02 | 6 |
| 4653 | N | TYR A 601 | 15.545 | 93.745 | 33.676 | 1.00 | 13.09 | 7 | 4695 | O ILE A 606 | 5.005 | 84.349 | 35.511 | 1.00 | 13.34 | 8 |
| 4654 | CA | TYR A 601 | 14.926 | 92.453 | 33.883 | 1.00 | 12.76 | 6 | 4696 | CB ILE A 606 | 2.995 | 83.184 | 33.259 | 1.00 | 11.81 | 6 |
| 4655 | C | TYR A 601 | 13.531 | 92.475 | 33.288 | 1.00 | 13.27 | 6 | 4697 | CG1 ILE A 606 | 4.029 | 83.874 | 32.346 | 1.00 | 12.94 | 6 |
| 4656 | O | TYR A 601 | 12.914 | 93.491 | 32.986 | 1.00 | 15.09 | 8 | 4698 | CG2 ILE A 606 | 1.625 | 83.138 | 32.550 | 1.00 | 15.56 | 6 |
| 4657 | CB | TYR A 601 | 14.751 | 92.119 | 35.387 | 1.00 | 14.11 | 6 | 4699 | CD1 ILE A 606 | 4.300 | 82.981 | 31.113 | 1.00 | 15.13 | 6 |
| 4658 | CG | TYR A 601 | 16.055 | 91.805 | 36.078 | 1.00 | 11.98 | 6 | 4700 | N PRO A 607 | 4.181 | 82.331 | 36.033 | 1.00 | 13.09 | 7 |
| 4659 | CD1 | TYR A 601 | 16.902 | 92.834 | 36.502 | 1.00 | 12.52 | 6 | 4701 | CA PRO A 607 | 5.294 | 81.982 | 36.937 | 1.00 | 12.68 | 6 |
| 4660 | CD2 | TYR A 601 | 16.473 | 90.490 | 36.242 | 1.00 | 12.95 | 6 | 4702 | C PRO A 607 | 6.616 | 81.880 | 36.189 | 1.00 | 10.98 | 6 |
| 4661 | CE1 | TYR A 601 | 18.138 | 92.544 | 37.097 | 1.00 | 13.54 | 6 | 4703 | O PRO A 607 | 7.700 | 82.258 | 36.671 | 1.00 | 14.73 | 8 |
| 4662 | CE2 | TYR A 601 | 17.673 | 90.213 | 36.888 | 1.00 | 14.26 | 6 | 4704 | CB PRO A 607 | 4.895 | 80.647 | 37.607 | 1.00 | 13.69 | 6 |
| 4663 | CZ | TYR A 601 | 18.499 | 91.239 | 37.276 | 1.00 | 15.84 | 6 | 4705 | CG PRO A 607 | 3.818 | 80.118 | 36.675 | 1.00 | 16.48 | 6 |
| 4664 | OH | TYR A 601 | 19.691 | 90.903 | 37.935 | 1.00 | 16.92 | 8 | 4706 | CD PRO A 607 | 3.081 | 81.335 | 36.098 | 1.00 | 16.43 | 6 |
| 4665 | N | LEU A 602 | 12.986 | 91.285 | 33.068 | 1.00 | 11.99 | 7 | 4707 | N GLU A 608 | 6.531 | 81.525 | 34.880 | 1.00 | 11.74 | 7 |
| 4666 | CA | LEU A 602 | 11.657 | 91.057 | 32.494 | 1.00 | 13.20 | 6 | 4708 | CA GLU A 608 | 7.747 | 81.559 | 34.031 | 1.00 | 10.58 | 6 |
| 4667 | C | LEU A 602 | 10.762 | 90.434 | 33.580 | 1.00 | 14.26 | 6 | 4709 | C GLU A 608 | 8.382 | 82.958 | 33.994 | 1.00 | 13.60 | 6 |
| 4668 | O | LEU A 602 | 11.148 | 89.522 | 34.284 | 1.00 | 13.06 | 8 | 4710 | O GLU A 608 | 9.606 | 83.060 | 33.731 | 1.00 | 11.79 | 8 |
| 4669 | CB | LEU A 602 | 11.794 | 90.060 | 31.334 | 1.00 | 13.29 | 6 | 4711 | CB GLU A 608 | 7.437 | 81.056 | 32.616 | 1.00 | 11.09 | 6 |
| 4670 | CG | LEU A 602 | 10.506 | 89.432 | 30.800 | 1.00 | 10.59 | 6 | 4712 | CG GLU A 608 | 7.145 | 79.550 | 32.522 | 1.00 | 10.94 | 6 |
| 4671 | CD1 | LEU A 602 | 9.579 | 90.481 | 30.155 | 1.00 | 14.08 | 6 | 4713 | CD GLU A 608 | 5.674 | 79.163 | 32.699 | 1.00 | 14.31 | 6 |
| 4672 | CD2 | LEU A 602 | 10.864 | 88.385 | 29.704 | 1.00 | 11.83 | 6 | 4714 | OE1 GLU A 608 | 4.875 | 79.973 | 33.221 | 1.00 | 12.87 | 8 |
| 4673 | CA | THR A 603 | 9.482 | 90.861 | 33.649 | 1.00 | 12.02 | 7 | 4715 | OE2 GLU A 608 | 5.344 | 78.040 | 32.280 | 1.00 | 13.22 | 8 |
| 4674 | N | THR A 603 | 8.570 | 90.233 | 34.635 | 1.00 | 12.81 | 6 | 4716 | N LEU A 609 | 7.571 | 83.999 | 34.112 | 1.00 | 11.31 | 7 |
| 4675 | C | THR A 603 | 7.158 | 90.267 | 34.066 | 1.00 | 12.50 | 6 | 4717 | CA LEU A 609 | 8.093 | 85.359 | 34.095 | 1.00 | 11.00 | 6 |
| 4676 | O | THR A 603 | 6.876 | 91.096 | 33.183 | 1.00 | 14.59 | 8 | 4718 | C LEU A 609 | 7.944 | 86.002 | 35.453 | 1.00 | 12.01 | 6 |
| 4677 | CB | THR A 603 | 8.711 | 90.983 | 35.969 | 1.00 | 14.38 | 6 | 4719 | O LEU A 609 | 7.959 | 87.224 | 35.602 | 1.00 | 14.24 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4720 | CB | LEU A 609 | 7.249 | 86.188 | 33.078 | 1.00 | 14.30 | 6 | 4762 | CG2 | THR A 614 | 9.718 | 94.523 | 40.520 | 1.00 | 18.09 | 6 |
| 4721 | CG | LEU A 609 | 7.424 | 85.668 | 31.627 | 1.00 | 13.57 | 6 | 4763 | N | ASP A 615 | 12.033 | 90.680 | 42.425 | 1.00 | 13.65 | 7 |
| 4722 | CD1 | LEU A 609 | 6.672 | 86.643 | 30.695 | 1.00 | 18.28 | 6 | 4764 | CA | ASP A 615 | 13.138 | 90.024 | 43.143 | 1.00 | 15.24 | 6 |
| 4723 | CD2 | LEU A 609 | 8.912 | 85.648 | 31.238 | 1.00 | 14.71 | 6 | 4765 | C | ASP A 615 | 14.084 | 89.416 | 42.093 | 1.00 | 12.74 | 6 |
| 4724 | N | GLY A 610 | 7.854 | 85.194 | 36.525 | 1.00 | 10.78 | 7 | 4766 | O | ASP A 615 | 13.582 | 88.794 | 41.143 | 1.00 | 13.71 | 8 |
| 4725 | CA | GLY A 610 | 7.950 | 85.729 | 37.864 | 1.00 | 10.94 | 6 | 4767 | CB | ASP A 615 | 12.511 | 88.981 | 44.075 | 1.00 | 14.77 | 6 |
| 4726 | C | GLY A 610 | 6.664 | 86.230 | 38.554 | 1.00 | 13.37 | 6 | 4768 | CG | ASP A 615 | 13.634 | 88.423 | 44.970 | 1.00 | 21.15 | 6 |
| 4727 | O | GLY A 610 | 6.767 | 86.832 | 39.647 | 1.00 | 13.90 | 8 | 4769 | OD1 | ASP A 615 | 13.956 | 88.932 | 46.048 | 1.00 | 23.65 | 8 |
| 4728 | N | ASN A 611 | 5.525 | 86.174 | 37.906 | 1.00 | 13.56 | 7 | 4770 | OD2 | ASP A 615 | 14.204 | 87.431 | 44.586 | 1.00 | 18.42 | 8 |
| 4729 | CA | ASN A 611 | 4.262 | 86.696 | 38.463 | 1.00 | 14.13 | 6 | 4771 | N | THR A 616 | 15.390 | 89.536 | 42.350 | 1.00 | 12.77 | 7 |
| 4730 | C | ASN A 611 | 4.462 | 88.079 | 39.072 | 1.00 | 13.68 | 6 | 4772 | CA | THR A 616 | 16.387 | 89.067 | 41.365 | 1.00 | 13.57 | 6 |
| 4731 | O | ASN A 611 | 4.063 | 88.427 | 40.207 | 1.00 | 14.78 | 8 | 4773 | C | THR A 616 | 17.391 | 88.146 | 42.072 | 1.00 | 15.88 | 6 |
| 4732 | CB | ASN A 611 | 3.695 | 85.782 | 39.555 | 1.00 | 13.73 | 6 | 4774 | O | THR A 616 | 18.487 | 87.902 | 41.566 | 1.00 | 14.89 | 8 |
| 4733 | CG | ASN A 611 | 3.110 | 84.538 | 38.890 | 1.00 | 16.98 | 6 | 4775 | CB | THR A 616 | 17.144 | 90.224 | 40.674 | 1.00 | 14.32 | 6 |
| 4734 | OD1 | ASN A 611 | 2.353 | 84.585 | 37.897 | 1.00 | 17.26 | 8 | 4776 | OG1 | THR A 616 | 17.752 | 91.045 | 41.713 | 1.00 | 15.99 | 8 |
| 4735 | ND2 | ASN A 611 | 3.501 | 83.420 | 39.478 | 1.00 | 16.08 | 7 | 4777 | CG2 | THR A 616 | 16.189 | 91.128 | 39.884 | 1.00 | 16.33 | 6 |
| 4736 | N | TRP A 612 | 5.010 | 88.962 | 38.242 | 1.00 | 13.00 | 7 | 4778 | N | SER A 617 | 16.981 | 87.590 | 43.216 | 1.00 | 13.15 | 7 |
| 4737 | CA | TRP A 612 | 5.298 | 90.339 | 38.534 | 1.00 | 13.35 | 6 | 4779 | CA | SER A 617 | 17.813 | 86.641 | 43.956 | 1.00 | 12.49 | 6 |
| 4738 | C | TRP A 612 | 6.284 | 90.676 | 39.608 | 1.00 | 14.25 | 6 | 4780 | C | SER A 617 | 17.759 | 85.265 | 43.312 | 1.00 | 13.68 | 6 |
| 4739 | O | TRP A 612 | 6.420 | 91.775 | 40.107 | 1.00 | 15.26 | 8 | 4781 | O | SER A 617 | 17.193 | 85.034 | 42.235 | 1.00 | 12.79 | 8 |
| 4740 | CB | TRP A 612 | 3.915 | 91.044 | 38.832 | 1.00 | 13.65 | 6 | 4782 | CB | SER A 617 | 17.271 | 86.583 | 45.396 | 1.00 | 14.38 | 6 |
| 4741 | CG | TRP A 612 | 2.965 | 91.036 | 37.664 | 1.00 | 13.25 | 6 | 4783 | OG | SER A 617 | 16.056 | 85.882 | 45.441 | 1.00 | 15.10 | 8 |
| 4742 | CD1 | TRP A 612 | 1.775 | 90.359 | 37.632 | 1.00 | 13.84 | 6 | 4784 | N | GLY A 618 | 18.327 | 84.268 | 44.080 | 1.00 | 15.05 | 7 |
| 4743 | CD2 | TRP A 612 | 3.138 | 91.564 | 36.359 | 1.00 | 14.07 | 6 | 4785 | CA | GLY A 618 | 18.300 | 82.869 | 43.621 | 1.00 | 13.01 | 6 |
| 4744 | NE1 | TRP A 612 | 1.160 | 90.489 | 36.402 | 1.00 | 13.90 | 7 | 4786 | C | GLY A 618 | 16.967 | 82.147 | 43.811 | 1.00 | 13.49 | 6 |
| 4745 | CE2 | TRP A 612 | 1.983 | 91.288 | 35.617 | 1.00 | 16.64 | 6 | 4787 | O | GLY A 618 | 16.835 | 80.938 | 43.552 | 1.00 | 15.47 | 8 |
| 4746 | CE3 | TRP A 612 | 4.148 | 92.402 | 35.815 | 1.00 | 15.91 | 6 | 4788 | N | ALA A 619 | 15.893 | 82.847 | 44.200 | 1.00 | 13.99 | 7 |
| 4747 | C22 | TRP A 612 | 1.843 | 91.676 | 34.288 | 1.00 | 14.35 | 6 | 4789 | CA | ALA A 619 | 14.592 | 82.218 | 44.333 | 1.00 | 14.93 | 6 |
| 4748 | C23 | TRP A 612 | 3.980 | 92.856 | 34.506 | 1.00 | 14.55 | 6 | 4790 | C | ALA A 619 | 14.033 | 81.691 | 43.015 | 1.00 | 15.28 | 6 |
| 4749 | CH2 | TRP A 612 | 2.844 | 92.490 | 33.747 | 1.00 | 14.05 | 6 | 4791 | O | ALA A 619 | 14.489 | 82.043 | 41.907 | 1.00 | 15.28 | 8 |
| 4750 | N | SER A 613 | 7.114 | 89.674 | 40.049 | 1.00 | 14.59 | 7 | 4792 | CB | ALA A 619 | 13.582 | 83.263 | 44.854 | 1.00 | 17.52 | 6 |
| 4751 | CA | SER A 613 | 8.136 | 89.943 | 41.025 | 1.00 | 16.76 | 6 | 4793 | N | VAL A 620 | 13.043 | 80.805 | 43.172 | 1.00 | 11.74 | 7 |
| 4752 | C | SER A 613 | 9.171 | 90.916 | 40.471 | 1.00 | 15.94 | 6 | 4794 | CA | VAL A 620 | 12.419 | 80.230 | 41.967 | 1.00 | 12.25 | 6 |
| 4753 | O | SER A 613 | 9.510 | 90.841 | 39.281 | 1.00 | 15.44 | 8 | 4795 | C | VAL A 620 | 11.259 | 81.126 | 41.502 | 1.00 | 12.14 | 6 |
| 4754 | CB | SER A 613 | 8.804 | 88.572 | 41.315 | 1.00 | 14.15 | 6 | 4796 | O | VAL A 620 | 10.533 | 81.679 | 42.344 | 1.00 | 14.38 | 8 |
| 4755 | OG | SER A 613 | 9.842 | 88.719 | 42.250 | 1.00 | 15.35 | 8 | 4797 | CB | VAL A 620 | 11.796 | 78.892 | 42.436 | 1.00 | 15.46 | 6 |
| 4756 | N | THR A 614 | 9.821 | 91.648 | 41.406 | 1.00 | 13.40 | 7 | 4798 | CG1 | VAL A 620 | 11.242 | 78.231 | 41.173 | 1.00 | 13.86 | 6 |
| 4757 | CA | THR A 614 | 11.021 | 92.394 | 41.037 | 1.00 | 13.18 | 6 | 4799 | CG2 | VAL A 620 | 12.924 | 77.941 | 42.923 | 1.00 | 15.04 | 6 |
| 4758 | C | THR A 614 | 12.238 | 91.869 | 41.796 | 1.00 | 12.85 | 6 | 4800 | N | ASN A 621 | 11.157 | 81.254 | 40.168 | 1.00 | 12.23 | 7 |
| 4759 | O | THR A 614 | 13.311 | 92.464 | 41.777 | 1.00 | 15.88 | 8 | 4801 | CA | ASN A 621 | 10.066 | 82.044 | 39.571 | 1.00 | 12.45 | 6 |
| 4760 | CB | THR A 614 | 10.895 | 93.904 | 41.297 | 1.00 | 16.41 | 6 | 4802 | C | ASN A 621 | 9.968 | 83.484 | 40.032 | 1.00 | 12.62 | 6 |
| 4761 | OG1 | THR A 614 | 10.626 | 94.073 | 42.724 | 1.00 | 18.07 | 8 | 4803 | O | ASN A 621 | 8.860 | 83.896 | 40.480 | 1.00 | 12.87 | 8 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 4804 | CB | ASN A 621 | 8.676 | 81.346 | 39.732 | 1.00 | 10.99 | 6 | 4846 | CG | LEU A 627 | 16.549 | 91.433 | 28.919 | 1.00 | 13.68 | 6 |
| 4805 | CG | ASN A 621 | 8.656 | 79.972 | 39.084 | 1.00 | 11.13 | 6 | 4847 | CD1 | LEU A 627 | 15.771 | 91.075 | 30.200 | 1.00 | 16.08 | 6 |
| 4806 | OD1 | ASN A 621 | 9.398 | 79.689 | 38.141 | 1.00 | 13.90 | 8 | 4848 | CD2 | LEU A 627 | 15.630 | 92.370 | 28.084 | 1.00 | 16.33 | 6 |
| 4807 | ND2 | ASN A 621 | 7.742 | 79.105 | 39.596 | 1.00 | 13.32 | 7 | 4849 | N | LEU A 628 | 20.804 | 91.374 | 28.421 | 1.00 | 12.55 | 7 |
| 4808 | N | ASN A 622 | 11.106 | 84.199 | 40.048 | 1.00 | 13.97 | 7 | 4850 | CA | LEU A 628 | 22.139 | 91.805 | 27.919 | 1.00 | 12.76 | 6 |
| 4809 | CA | ASN A 622 | 11.116 | 85.623 | 40.322 | 1.00 | 11.35 | 6 | 4851 | C | LEU A 628 | 21.994 | 92.999 | 26.973 | 1.00 | 15.67 | 6 |
| 4810 | C | ASN A 622 | 11.418 | 86.389 | 39.037 | 1.00 | 12.47 | 6 | 4852 | O | LEU A 628 | 20.910 | 93.197 | 26.394 | 1.00 | 14.76 | 8 |
| 4811 | O | ASN A 622 | 11.090 | 85.862 | 37.960 | 1.00 | 12.66 | 8 | 4853 | CB | LEU A 628 | 22.746 | 90.663 | 27.111 | 1.00 | 14.06 | 6 |
| 4812 | CB | ASN A 622 | 12.073 | 85.956 | 41.471 | 1.00 | 12.54 | 6 | 4854 | CG | LEU A 628 | 22.848 | 89.332 | 27.886 | 1.00 | 14.72 | 6 |
| 4813 | CG | ASN A 622 | 13.543 | 85.545 | 41.151 | 1.00 | 12.82 | 6 | 4855 | CD1 | LEU A 628 | 23.526 | 88.239 | 27.056 | 1.00 | 12.14 | 6 |
| 4814 | OD1 | ASN A 622 | 13.811 | 85.093 | 40.044 | 1.00 | 12.70 | 8 | 4856 | CD2 | LEU A 628 | 23.659 | 89.508 | 29.185 | 1.00 | 20.12 | 6 |
| 4815 | ND2 | ASN A 622 | 14.377 | 85.753 | 42.196 | 1.00 | 13.72 | 7 | 4857 | N | ALA A 629 | 23.117 | 93.699 | 26.702 | 1.00 | 16.33 | 7 |
| 4816 | N | ALA A 623 | 11.883 | 87.626 | 39.098 | 1.00 | 11.27 | 7 | 4858 | CA | ALA A 629 | 22.871 | 94.875 | 25.787 | 1.00 | 16.83 | 6 |
| 4817 | CA | ALA A 623 | 12.088 | 88.339 | 37.812 | 1.00 | 12.38 | 6 | 4859 | C | ALA A 629 | 23.983 | 95.083 | 24.795 | 1.00 | 15.77 | 6 |
| 4818 | C | ALA A 623 | 13.107 | 87.592 | 36.947 | 1.00 | 13.25 | 6 | 4860 | O | ALA A 629 | 24.610 | 96.177 | 24.707 | 1.00 | 15.92 | 8 |
| 4819 | O | ALA A 623 | 14.035 | 87.018 | 37.469 | 1.00 | 13.43 | 8 | 4861 | CB | ALA A 629 | 22.674 | 96.098 | 26.674 | 1.00 | 15.56 | 6 |
| 4820 | CB | ALA A 623 | 12.586 | 89.748 | 38.120 | 1.00 | 14.46 | 6 | 4862 | N | PRO A 630 | 24.278 | 94.136 | 23.970 | 1.00 | 16.96 | 7 |
| 4821 | N | GLN A 624 | 12.905 | 87.740 | 35.631 | 1.00 | 12.11 | 7 | 4863 | CA | PRO A 630 | 25.237 | 94.281 | 22.873 | 1.00 | 19.28 | 6 |
| 4822 | CA | GLN A 624 | 13.742 | 87.034 | 34.660 | 1.00 | 11.87 | 6 | 4864 | C | PRO A 630 | 24.773 | 95.400 | 21.940 | 1.00 | 21.06 | 6 |
| 4823 | C | GLN A 624 | 14.828 | 87.912 | 34.071 | 1.00 | 12.70 | 6 | 4865 | O | PRO A 630 | 25.633 | 96.015 | 21.314 | 1.00 | 23.58 | 8 |
| 4824 | O | GLN A 624 | 14.646 | 89.092 | 33.762 | 1.00 | 13.14 | 8 | 4866 | CB | PRO A 630 | 25.314 | 92.944 | 22.123 | 1.00 | 17.59 | 6 |
| 4825 | CB | GLN A 624 | 12.880 | 86.477 | 33.521 | 1.00 | 14.55 | 6 | 4867 | CG | PRO A 630 | 23.928 | 92.367 | 22.442 | 1.00 | 18.42 | 6 |
| 4826 | CG | GLN A 624 | 11.779 | 85.492 | 34.084 | 1.00 | 13.33 | 6 | 4868 | CD | PRO A 630 | 23.644 | 92.807 | 23.877 | 1.00 | 18.05 | 6 |
| 4827 | CD | GLN A 624 | 12.451 | 84.323 | 34.754 | 1.00 | 14.35 | 6 | 4869 | N | ASN A 631 | 23.464 | 95.562 | 21.768 | 1.00 | 17.93 | 7 |
| 4828 | OE1 | GLN A 624 | 13.213 | 83.546 | 34.096 | 1.00 | 15.81 | 8 | 4870 | CA | ASN A 631 | 22.935 | 96.635 | 20.926 | 1.00 | 17.58 | 6 |
| 4829 | NE2 | GLN A 624 | 12.268 | 84.078 | 36.040 | 1.00 | 14.08 | 7 | 4871 | C | ASN A 631 | 22.382 | 97.779 | 21.748 | 1.00 | 17.45 | 6 |
| 4830 | N | GLY A 625 | 15.989 | 87.264 | 33.941 | 1.00 | 12.93 | 7 | 4872 | O | ASN A 631 | 21.359 | 98.370 | 21.354 | 1.00 | 18.41 | 8 |
| 4831 | CA | GLY A 625 | 17.183 | 87.950 | 33.418 | 1.00 | 12.61 | 6 | 4873 | CB | ASN A 631 | 21.902 | 96.082 | 19.950 | 1.00 | 18.61 | 6 |
| 4832 | C | GLY A 625 | 18.392 | 87.917 | 34.310 | 1.00 | 12.24 | 6 | 4874 | CG | ASN A 631 | 22.400 | 94.876 | 19.161 | 1.00 | 28.21 | 6 |
| 4833 | O | GLY A 625 | 18.497 | 86.888 | 34.934 | 1.00 | 13.82 | 8 | 4875 | OD1 | ASN A 631 | 21.838 | 93.764 | 19.168 | 1.00 | 27.73 | 8 |
| 4834 | N | PRO A 626 | 19.296 | 88.815 | 34.131 | 1.00 | 12.81 | 7 | 4876 | ND2 | ASN A 631 | 23.476 | 95.224 | 18.455 | 1.00 | 17.84 | 7 |
| 4835 | CA | PRO A 626 | 19.237 | 90.097 | 33.510 | 1.00 | 15.64 | 6 | 4877 | N | TYR A 632 | 22.980 | 98.110 | 22.883 | 1.00 | 16.27 | 7 |
| 4836 | C | PRO A 626 | 19.288 | 89.998 | 32.003 | 1.00 | 15.42 | 6 | 4878 | CA | TYR A 632 | 22.570 | 99.229 | 23.700 | 1.00 | 17.84 | 6 |
| 4837 | O | PRO A 626 | 19.675 | 88.992 | 31.364 | 1.00 | 15.65 | 8 | 4879 | C | TYR A 632 | 22.255 | 100.496 | 22.909 | 1.00 | 19.89 | 6 |
| 4838 | CB | PRO A 626 | 20.374 | 91.012 | 34.019 | 1.00 | 15.71 | 6 | 4880 | O | TYR A 632 | 23.030 | 100.672 | 21.982 | 1.00 | 19.89 | 8 |
| 4839 | CG | PRO A 626 | 21.401 | 89.927 | 34.320 | 1.00 | 14.63 | 6 | 4881 | CB | TYR A 632 | 23.749 | 99.537 | 24.643 | 1.00 | 18.23 | 6 |
| 4840 | CD | PRO A 626 | 20.565 | 88.780 | 34.858 | 1.00 | 13.83 | 6 | 4882 | CG | TYR A 632 | 23.520 | 100.604 | 25.654 | 1.00 | 20.78 | 6 |
| 4841 | N | LEU A 627 | 18.725 | 91.061 | 29.381 | 1.00 | 13.98 | 7 | 4883 | CD1 | TYR A 632 | 22.919 | 100.369 | 26.875 | 1.00 | 20.07 | 6 |
| 4842 | CA | LEU A 627 | 18.935 | 91.116 | 29.881 | 1.00 | 13.16 | 6 | 4884 | CD2 | TYR A 632 | 23.839 | 101.933 | 25.333 | 1.00 | 22.98 | 6 |
| 4843 | C | LEU A 627 | 20.364 | 91.609 | 29.649 | 1.00 | 14.14 | 6 | 4885 | CE1 | TYR A 632 | 22.700 | 101.367 | 27.797 | 1.00 | 22.62 | 6 |
| 4844 | O | LEU A 627 | 21.024 | 92.215 | 30.527 | 1.00 | 14.86 | 8 | 4886 | CE2 | TYR A 632 | 23.578 | 102.953 | 26.223 | 1.00 | 23.64 | 6 |
| 4845 | CB | LEU A 627 | 17.906 | 92.080 | 29.214 | 1.00 | 13.73 | 6 | 4887 | CZ | TYR A 632 | 23.051 | 102.671 | 27.457 | 1.00 | 27.32 | 6 |

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|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4888 | OH | TYR A 632 | 22.814 | 103.670 | 28.369 | 1.00 | 23.27 | 8 | 4930 | CA | TYR A 637 | 17.759 | 87.841 | 26.425 | 1.00 | 12.35 | 6 |
| 4889 | N | PRO A 633 | 21.113 | 101.067 | 23.157 | 1.00 | 19.06 | 7 | 4931 | C | TYR A 637 | 16.714 | 86.848 | 25.989 | 1.00 | 12.24 | 6 |
| 4890 | CA | PRO A 633 | 20.194 | 101.103 | 24.225 | 1.00 | 16.58 | 6 | 4932 | O | TYR A 637 | 15.911 | 87.135 | 25.088 | 1.00 | 12.49 | 8 |
| 4891 | C | PRO A 633 | 19.087 | 100.033 | 24.123 | 1.00 | 15.76 | 6 | 4933 | CB | TYR A 637 | 18.183 | 87.770 | 27.903 | 1.00 | 12.77 | 6 |
| 4892 | O | PRO A 633 | 18.188 | 100.153 | 24.954 | 1.00 | 16.24 | 8 | 4934 | CG | TYR A 637 | 19.035 | 86.513 | 28.195 | 1.00 | 13.33 | 6 |
| 4893 | CB | PRO A 633 | 19.474 | 102.498 | 24.311 | 1.00 | 19.94 | 6 | 4935 | CD1 | TYR A 637 | 20.253 | 86.244 | 27.548 | 1.00 | 12.60 | 6 |
| 4894 | CG | PRO A 633 | 19.449 | 102.810 | 22.846 | 1.00 | 24.00 | 6 | 4936 | CD2 | TYR A 637 | 18.595 | 85.573 | 29.127 | 1.00 | 10.55 | 6 |
| 4895 | CD | PRO A 633 | 20.772 | 102.271 | 22.369 | 1.00 | 24.76 | 6 | 4937 | CE1 | TYR A 637 | 21.022 | 85.134 | 27.792 | 1.00 | 11.85 | 6 |
| 4896 | N | ASP A 634 | 19.272 | 99.094 | 23.169 | 1.00 | 16.18 | 7 | 4938 | CE2 | TYR A 637 | 19.321 | 84.424 | 29.387 | 1.00 | 12.60 | 6 |
| 4897 | CA | ASP A 634 | 18.330 | 97.978 | 23.121 | 1.00 | 16.48 | 6 | 4939 | CZ | TYR A 637 | 20.521 | 84.221 | 28.728 | 1.00 | 11.69 | 6 |
| 4898 | C | ASP A 634 | 18.923 | 96.792 | 23.937 | 1.00 | 15.97 | 6 | 4940 | OH | TYR A 637 | 21.255 | 83.073 | 29.016 | 1.00 | 11.85 | 8 |
| 4899 | O | ASP A 634 | 20.153 | 96.671 | 24.058 | 1.00 | 16.27 | 8 | 4941 | N | VAL A 638 | 16.857 | 85.565 | 26.379 | 1.00 | 12.66 | 7 |
| 4900 | CB | ASP A 634 | 18.133 | 97.402 | 21.731 | 1.00 | 15.05 | 6 | 4942 | CA | VAL A 638 | 16.033 | 84.508 | 25.827 | 1.00 | 10.90 | 6 |
| 4901 | CG | ASP A 634 | 17.626 | 98.434 | 20.695 | 1.00 | 20.07 | 6 | 4943 | C | VAL A 638 | 15.492 | 83.693 | 27.023 | 1.00 | 11.04 | 6 |
| 4902 | OD1 | ASP A 634 | 17.138 | 99.519 | 21.100 | 1.00 | 17.34 | 8 | 4944 | O | VAL A 638 | 16.202 | 83.367 | 27.980 | 1.00 | 13.35 | 8 |
| 4903 | OD2 | ASP A 634 | 17.728 | 98.097 | 19.503 | 1.00 | 19.32 | 8 | 4945 | CB | VAL A 638 | 16.830 | 83.496 | 24.987 | 1.00 | 12.00 | 6 |
| 4904 | N | TRP A 635 | 18.009 | 96.147 | 24.656 | 1.00 | 14.45 | 7 | 4946 | CG1 | VAL A 638 | 15.922 | 82.650 | 24.118 | 1.00 | 12.74 | 6 |
| 4905 | CA | TRP A 635 | 18.413 | 95.017 | 25.510 | 1.00 | 16.15 | 6 | 4947 | CG2 | VAL A 638 | 17.799 | 84.300 | 24.074 | 1.00 | 10.59 | 6 |
| 4906 | C | TRP A 635 | 17.708 | 93.736 | 25.082 | 1.00 | 13.84 | 6 | 4948 | N | PHE A 639 | 14.137 | 83.517 | 26.957 | 1.00 | 12.77 | 7 |
| 4907 | O | TRP A 635 | 16.590 | 93.820 | 24.606 | 1.00 | 13.90 | 8 | 4949 | CA | PHE A 639 | 13.441 | 82.960 | 28.082 | 1.00 | 9.34 | 6 |
| 4908 | CB | TRP A 635 | 18.024 | 95.299 | 26.962 | 1.00 | 15.52 | 6 | 4950 | C | PHE A 639 | 12.466 | 81.877 | 27.665 | 1.00 | 11.56 | 6 |
| 4909 | CG | TRP A 635 | 18.818 | 96.421 | 27.587 | 1.00 | 14.07 | 6 | 4951 | O | PHE A 639 | 11.814 | 81.982 | 26.632 | 1.00 | 12.26 | 8 |
| 4910 | CD1 | TRP A 635 | 18.737 | 97.739 | 27.178 | 1.00 | 14.13 | 6 | 4952 | CB | PHE A 639 | 12.612 | 84.072 | 28.807 | 1.00 | 11.50 | 6 |
| 4911 | CD2 | TRP A 635 | 19.713 | 96.407 | 28.694 | 1.00 | 16.17 | 6 | 4953 | CG | PHE A 639 | 13.498 | 85.209 | 29.322 | 1.00 | 12.29 | 6 |
| 4912 | NE1 | TRP A 635 | 19.561 | 98.533 | 27.989 | 1.00 | 15.61 | 7 | 4954 | CD1 | PHE A 639 | 14.294 | 85.042 | 30.446 | 1.00 | 11.38 | 6 |
| 4913 | CE2 | TRP A 635 | 20.179 | 97.706 | 28.908 | 1.00 | 17.77 | 6 | 4955 | CD2 | PHE A 639 | 13.567 | 86.380 | 28.563 | 1.00 | 13.67 | 6 |
| 4914 | CE3 | TRP A 635 | 20.179 | 95.350 | 29.511 | 1.00 | 18.51 | 6 | 4956 | CE1 | PHE A 639 | 15.176 | 86.094 | 30.829 | 1.00 | 12.05 | 6 |
| 4915 | CZ2 | TRP A 635 | 21.071 | 98.018 | 29.935 | 1.00 | 19.26 | 6 | 4957 | CE2 | PHE A 639 | 14.416 | 87.425 | 28.965 | 1.00 | 13.84 | 6 |
| 4916 | CZ3 | TRP A 635 | 21.100 | 95.671 | 30.515 | 1.00 | 23.17 | 6 | 4958 | CZ | PHE A 639 | 15.196 | 87.301 | 30.113 | 1.00 | 13.28 | 6 |
| 4917 | CH2 | TRP A 635 | 21.514 | 96.992 | 30.735 | 1.00 | 20.92 | 6 | 4959 | N | SER A 640 | 12.323 | 80.913 | 28.609 | 1.00 | 10.61 | 7 |
| 4918 | N | PHE A 636 | 18.294 | 92.561 | 25.372 | 1.00 | 12.41 | 7 | 4960 | CA | SER A 640 | 11.376 | 79.833 | 28.360 | 1.00 | 11.72 | 6 |
| 4919 | CA | PHE A 636 | 17.562 | 91.335 | 24.947 | 1.00 | 11.57 | 6 | 4961 | C | SER A 640 | 10.005 | 80.223 | 28.872 | 1.00 | 11.19 | 6 |
| 4920 | O | PHE A 636 | 18.071 | 90.194 | 25.855 | 1.00 | 12.41 | 6 | 4962 | O | SER A 640 | 9.878 | 80.649 | 30.026 | 1.00 | 12.90 | 8 |
| 4921 | C | PHE A 636 | 19.204 | 90.239 | 26.345 | 1.00 | 13.24 | 8 | 4963 | CB | SER A 640 | 11.915 | 78.568 | 29.132 | 1.00 | 12.23 | 6 |
| 4922 | CB | PHE A 636 | 17.761 | 90.971 | 23.435 | 1.00 | 12.03 | 6 | 4964 | OG | SER A 640 | 11.028 | 77.448 | 28.846 | 1.00 | 12.04 | 8 |
| 4923 | CG | PHE A 636 | 19.030 | 90.118 | 23.261 | 1.00 | 12.15 | 6 | 4965 | N | VAL A 641 | 9.007 | 80.190 | 27.975 | 1.00 | 8.82 | 7 |
| 4924 | CD1 | PHE A 636 | 20.287 | 90.667 | 23.292 | 1.00 | 17.38 | 6 | 4966 | CA | VAL A 641 | 7.635 | 80.609 | 28.374 | 1.00 | 11.37 | 6 |
| 4925 | CD2 | PHE A 636 | 18.856 | 88.751 | 23.095 | 1.00 | 11.02 | 6 | 4967 | C | VAL A 641 | 6.697 | 79.601 | 27.775 | 1.00 | 11.35 | 6 |
| 4926 | CE1 | PHE A 636 | 21.417 | 89.860 | 23.207 | 1.00 | 19.56 | 6 | 4968 | O | VAL A 641 | 7.075 | 78.840 | 26.864 | 1.00 | 10.31 | 8 |
| 4927 | CE2 | PHE A 636 | 19.996 | 87.906 | 22.997 | 1.00 | 12.49 | 6 | 4969 | CB | VAL A 641 | 7.286 | 82.019 | 27.760 | 1.00 | 11.50 | 6 |
| 4928 | CZ | PHE A 636 | 21.250 | 88.466 | 23.034 | 1.00 | 17.21 | 6 | 4970 | CG1 | VAL A 641 | 8.061 | 83.038 | 28.624 | 1.00 | 13.20 | 6 |
| 4929 | N | TYR A 637 | 17.229 | 89.170 | 25.966 | 1.00 | 12.09 | 7 | 4971 | CG2 | VAL A 641 | 7.607 | 82.115 | 26.241 | 1.00 | 10.82 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 4972 | N | PRO A 642 | 5.470 | 79.384 | 28.254 | 1.00 | 10.92 | 7 | 5014 | C | GLN A 648 | 2.687 | 90.407 | 30.490 | 1.00 | 15.15 | 6 |
| 4973 | CA | PRO A 642 | 4.582 | 78.438 | 27.626 | 1.00 | 11.56 | 6 | 5015 | O | GLN A 648 | 3.041 | 89.586 | 31.338 | 1.00 | 15.89 | 8 |
| 4974 | C | PRO A 642 | 4.256 | 78.780 | 26.166 | 1.00 | 10.87 | 6 | 5016 | CB | GLN A 648 | 0.298 | 90.835 | 30.611 | 1.00 | 13.04 | 6 |
| 4975 | O | PRO A 642 | 4.048 | 79.994 | 25.888 | 1.00 | 12.26 | 8 | 5017 | CG | GLN A 648 | -1.032 | 90.704 | 29.820 | 1.00 | 20.15 | 6 |
| 4976 | CB | PRO A 642 | 3.295 | 78.524 | 28.529 | 1.00 | 11.37 | 6 | 5018 | CD | GLN A 648 | -2.040 | 91.727 | 30.260 | 1.00 | 27.13 | 6 |
| 4977 | CG | PRO A 642 | 3.352 | 79.948 | 29.064 | 1.00 | 11.52 | 6 | 5019 | OE1 | GLN A 648 | -1.797 | 92.691 | 30.982 | 1.00 | 23.22 | 8 |
| 4978 | CD | PRO A 642 | 4.866 | 80.234 | 29.308 | 1.00 | 14.12 | 6 | 5020 | NE2 | GLN A 648 | -3.309 | 91.503 | 29.847 | 1.00 | 28.35 | 7 |
| 4979 | N | ALA A 643 | 4.267 | 77.800 | 25.291 | 1.00 | 11.34 | 7 | 5021 | N | PHE A 649 | 3.446 | 91.461 | 30.155 | 1.00 | 13.26 | 7 |
| 4980 | CA | ALA A 643 | 4.033 | 77.992 | 23.839 | 1.00 | 12.12 | 6 | 5022 | CA | PHE A 649 | 4.767 | 91.622 | 30.746 | 1.00 | 12.72 | 6 |
| 4981 | C | ALA A 643 | 2.531 | 78.215 | 23.567 | 1.00 | 13.78 | 6 | 5023 | C | PHE A 649 | 5.219 | 93.094 | 30.663 | 1.00 | 14.64 | 6 |
| 4982 | O | ALA A 643 | 1.681 | 77.650 | 24.236 | 1.00 | 15.31 | 8 | 5024 | O | PHE A 649 | 4.697 | 93.903 | 29.862 | 1.00 | 14.50 | 8 |
| 4983 | CB | ALA A 643 | 4.330 | 76.657 | 23.141 | 1.00 | 13.71 | 6 | 5025 | CB | PHE A 649 | 5.812 | 90.743 | 30.051 | 1.00 | 12.47 | 6 |
| 4984 | N | GLY A 644 | 2.317 | 79.106 | 22.623 | 1.00 | 14.27 | 7 | 5026 | CG | PHE A 649 | 5.875 | 90.962 | 28.544 | 1.00 | 13.33 | 6 |
| 4985 | CA | GLY A 644 | 0.952 | 79.377 | 22.150 | 1.00 | 14.42 | 6 | 5027 | CD1 | PHE A 649 | 4.996 | 90.400 | 27.682 | 1.00 | 14.84 | 6 |
| 4986 | C | GLY A 644 | 0.065 | 80.108 | 23.133 | 1.00 | 15.94 | 6 | 5028 | CD2 | PHE A 649 | 6.861 | 91.790 | 28.013 | 1.00 | 13.41 | 6 |
| 4987 | O | GLY A 644 | -1.154 | 79.765 | 23.178 | 1.00 | 19.30 | 8 | 5029 | CE1 | PHE A 649 | 5.031 | 90.678 | 26.303 | 1.00 | 15.17 | 6 |
| 4988 | N | LYS A 645 | 0.597 | 80.884 | 24.030 | 1.00 | 14.60 | 7 | 5030 | CE2 | PHE A 649 | 6.977 | 92.043 | 26.666 | 1.00 | 16.16 | 6 |
| 4989 | CA | LYS A 645 | -0.171 | 81.519 | 25.092 | 1.00 | 14.20 | 6 | 5031 | CZ | PHE A 649 | 6.057 | 91.493 | 25.807 | 1.00 | 13.88 | 6 |
| 4990 | C | LYS A 645 | -0.060 | 83.017 | 24.926 | 1.00 | 17.57 | 6 | 5032 | N | LYS A 650 | 6.135 | 93.413 | 31.538 | 1.00 | 13.99 | 7 |
| 4991 | O | LYS A 645 | 1.002 | 83.579 | 24.623 | 1.00 | 17.47 | 8 | 5033 | CA | LYS A 650 | 6.876 | 94.683 | 31.405 | 1.00 | 13.18 | 6 |
| 4992 | CB | LYS A 645 | 0.376 | 81.126 | 26.483 | 1.00 | 14.57 | 6 | 5034 | C | LYS A 650 | 8.349 | 94.411 | 31.797 | 1.00 | 15.87 | 6 |
| 4993 | CG | LYS A 645 | 0.313 | 79.611 | 26.725 | 1.00 | 17.45 | 6 | 5035 | O | LYS A 650 | 8.696 | 93.364 | 32.375 | 1.00 | 13.96 | 8 |
| 4994 | CD | LYS A 645 | -1.136 | 79.116 | 26.699 | 1.00 | 17.54 | 6 | 5036 | CB | LYS A 650 | 6.358 | 95.735 | 32.410 | 1.00 | 14.62 | 6 |
| 4995 | CE | LYS A 645 | -1.184 | 77.572 | 26.837 | 1.00 | 21.59 | 6 | 5037 | CG | LYS A 650 | 5.004 | 96.385 | 31.989 | 1.00 | 15.36 | 6 |
| 4996 | NZ | LYS A 645 | -0.587 | 77.121 | 28.112 | 1.00 | 31.91 | 7 | 5038 | CD | LYS A 650 | 4.922 | 97.604 | 32.979 | 1.00 | 19.44 | 6 |
| 4997 | N | THR A 646 | -1.157 | 83.717 | 25.357 | 1.00 | 14.42 | 7 | 5039 | CE | LYS A 650 | 3.841 | 98.565 | 32.553 | 1.00 | 24.45 | 6 |
| 4998 | CA | THR A 646 | -1.090 | 85.140 | 25.434 | 1.00 | 14.66 | 6 | 5040 | NZ | LYS A 650 | 3.898 | 99.741 | 33.515 | 1.00 | 18.41 | 7 |
| 4999 | C | THR A 646 | -0.662 | 85.594 | 26.824 | 1.00 | 13.55 | 6 | 5041 | N | PHE A 651 | 9.172 | 95.398 | 31.438 | 1.00 | 13.40 | 7 |
| 5000 | O | THR A 646 | -1.221 | 85.157 | 27.850 | 1.00 | 16.55 | 8 | 5042 | CA | PHE A 651 | 10.571 | 95.420 | 31.850 | 1.00 | 14.23 | 6 |
| 5001 | CB | THR A 646 | -2.510 | 85.720 | 25.098 | 1.00 | 17.00 | 6 | 5043 | C | PHE A 651 | 10.800 | 96.474 | 32.926 | 1.00 | 16.48 | 6 |
| 5002 | OG1 | THR A 646 | -2.824 | 85.361 | 23.738 | 1.00 | 16.76 | 8 | 5044 | O | PHE A 651 | 9.990 | 97.396 | 33.132 | 1.00 | 17.07 | 8 |
| 5003 | CG2 | THR A 646 | -2.463 | 87.240 | 25.195 | 1.00 | 18.18 | 6 | 5045 | CB | PHE A 651 | 11.465 | 95.783 | 30.638 | 1.00 | 12.48 | 6 |
| 5004 | N | ILE A 647 | 0.360 | 86.434 | 26.913 | 1.00 | 11.81 | 7 | 5046 | CG | PHE A 651 | 11.280 | 94.796 | 29.512 | 1.00 | 15.91 | 6 |
| 5005 | CA | ILE A 647 | 1.001 | 86.816 | 28.152 | 1.00 | 11.47 | 6 | 5047 | CD1 | PHE A 651 | 10.277 | 94.943 | 28.564 | 1.00 | 13.76 | 6 |
| 5006 | C | ILE A 647 | 1.047 | 88.357 | 28.250 | 1.00 | 13.84 | 6 | 5048 | CD2 | PHE A 651 | 12.127 | 93.681 | 29.453 | 1.00 | 14.89 | 6 |
| 5007 | O | ILE A 647 | 0.991 | 89.054 | 27.201 | 1.00 | 14.89 | 8 | 5049 | CE1 | PHE A 651 | 10.114 | 94.016 | 27.568 | 1.00 | 12.48 | 6 |
| 5008 | CB | ILE A 647 | 2.476 | 86.353 | 28.278 | 1.00 | 13.09 | 6 | 5050 | CE2 | PHE A 651 | 11.957 | 92.759 | 28.426 | 1.00 | 13.50 | 6 |
| 5009 | CG1 | ILE A 647 | 3.296 | 86.770 | 27.045 | 1.00 | 12.50 | 6 | 5051 | CZ | PHE A 651 | 10.944 | 92.884 | 27.461 | 1.00 | 16.56 | 6 |
| 5010 | CG2 | ILE A 647 | 2.410 | 84.817 | 28.343 | 1.00 | 14.24 | 6 | 5052 | N | PHE A 652 | 11.849 | 96.240 | 33.723 | 1.00 | 15.18 | 7 |
| 5011 | CD1 | ILE A 647 | 4.813 | 86.486 | 27.247 | 1.00 | 17.78 | 6 | 5053 | CA | PHE A 652 | 12.249 | 97.256 | 34.704 | 1.00 | 14.29 | 6 |
| 5012 | N | GLN A 648 | 1.150 | 88.776 | 29.495 | 1.00 | 12.61 | 7 | 5054 | C | PHE A 652 | 13.756 | 97.339 | 34.785 | 1.00 | 17.92 | 6 |
| 5013 | CA | GLN A 648 | 1.402 | 90.212 | 29.726 | 1.00 | 11.91 | 6 | 5055 | O | PHE A 652 | 14.452 | 96.365 | 34.487 | 1.00 | 15.37 | 8 |

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|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 5056 | CB | PHE A 652 | 11.634 | 96.950 | 36.084 | 1.00 | 15.14 | 6 | 5098 | C | ASP A 657 | 20.617 | 99.783 | 44.694 | 1.00 | 33.22 | 6 |
| 5057 | CG | PHE A 652 | 12.097 | 95.688 | 36.789 | 1.00 | 16.77 | 6 | 5099 | O | ASP A 657 | 20.202 | 99.906 | 45.852 | 1.00 | 30.17 | 8 |
| 5058 | CD1 | PHE A 652 | 13.251 | 95.685 | 37.565 | 1.00 | 15.74 | 6 | 5100 | CB | ASP A 657 | 21.725 | 102.050 | 44.643 | 1.00 | 27.78 | 6 |
| 5059 | CD2 | PHE A 652 | 11.326 | 94.553 | 36.695 | 1.00 | 15.90 | 6 | 5101 | CG | ASP A 657 | 20.499 | 102.712 | 44.087 | 1.00 | 34.66 | 6 |
| 5060 | CE1 | PHE A 652 | 13.633 | 94.518 | 38.231 | 1.00 | 14.76 | 6 | 5102 | OD1 | ASP A 657 | 19.665 | 102.035 | 43.431 | 1.00 | 28.22 | 8 |
| 5061 | CE2 | PHE A 652 | 11.695 | 93.407 | 37.380 | 1.00 | 15.19 | 6 | 5103 | OD2 | ASP A 657 | 20.239 | 103.920 | 44.267 | 1.00 | 33.52 | 8 |
| 5062 | CZ | PHE A 652 | 12.866 | 93.343 | 38.139 | 1.00 | 14.25 | 6 | 5104 | N | GLY A 658 | 20.019 | 98.958 | 43.803 | 1.00 | 29.54 | 7 |
| 5063 | N | ILE A 653 | 14.244 | 98.512 | 35.189 | 1.00 | 14.94 | 7 | 5105 | CA | GLY A 658 | 18.874 | 98.181 | 44.227 | 1.00 | 29.70 | 6 |
| 5064 | CA | ILE A 653 | 15.705 | 98.598 | 35.463 | 1.00 | 14.72 | 6 | 5106 | C | GLY A 658 | 17.543 | 98.837 | 43.931 | 1.00 | 26.81 | 6 |
| 5065 | C | ILE A 653 | 15.906 | 98.394 | 36.962 | 1.00 | 18.67 | 6 | 5107 | O | GLY A 658 | 16.531 | 98.126 | 43.935 | 1.00 | 30.39 | 8 |
| 5066 | O | ILE A 653 | 15.175 | 98.971 | 37.804 | 1.00 | 19.59 | 8 | 5108 | N | THR A 659 | 17.502 | 100.106 | 43.566 | 1.00 | 23.52 | 7 |
| 5067 | CB | ILE A 653 | 16.168 | 100.071 | 35.163 | 1.00 | 14.73 | 6 | 5109 | CA | THR A 659 | 16.313 | 100.826 | 43.215 | 1.00 | 25.61 | 6 |
| 5068 | CG1 | ILE A 653 | 16.000 | 100.337 | 33.693 | 1.00 | 18.74 | 6 | 5110 | C | THR A 659 | 15.641 | 100.184 | 41.985 | 1.00 | 23.40 | 6 |
| 5069 | CG2 | ILE A 653 | 17.628 | 100.201 | 35.616 | 1.00 | 18.25 | 6 | 5111 | O | THR A 659 | 16.419 | 99.778 | 41.118 | 1.00 | 27.85 | 8 |
| 5070 | CD1 | ILE A 653 | 16.191 | 101.838 | 33.353 | 1.00 | 20.43 | 6 | 5112 | CB | THR A 659 | 16.614 | 102.279 | 42.717 | 1.00 | 19.42 | 6 |
| 5071 | N | LYS A 654 | 16.847 | 97.524 | 37.282 | 1.00 | 17.58 | 7 | 5113 | OG1 | THR A 659 | 17.524 | 102.993 | 43.510 | 1.00 | 46.62 | 8 |
| 5072 | CA | LYS A 654 | 17.273 | 97.382 | 38.690 | 1.00 | 18.28 | 6 | 5114 | CG2 | THR A 659 | 15.276 | 103.016 | 42.706 | 1.00 | 37.02 | 6 |
| 5073 | C | LYS A 654 | 18.623 | 98.139 | 38.780 | 1.00 | 15.87 | 6 | 5115 | N | ILE A 660 | 14.319 | 100.215 | 41.909 | 1.00 | 20.34 | 7 |
| 5074 | O | LYS A 654 | 19.571 | 97.760 | 38.135 | 1.00 | 18.77 | 8 | 5116 | CA | ILE A 660 | 13.596 | 99.691 | 40.758 | 1.00 | 25.29 | 6 |
| 5075 | CB | LYS A 654 | 17.469 | 95.933 | 39.131 | 1.00 | 16.77 | 6 | 5117 | C | ILE A 660 | 12.933 | 100.761 | 39.919 | 1.00 | 25.57 | 6 |
| 5076 | CG | LYS A 654 | 17.774 | 95.976 | 40.661 | 1.00 | 20.67 | 6 | 5118 | O | ILE A 660 | 12.186 | 101.612 | 40.465 | 1.00 | 27.02 | 8 |
| 5077 | CD | LYS A 654 | 17.709 | 94.558 | 41.235 | 1.00 | 24.12 | 6 | 5119 | CB | ILE A 660 | 12.458 | 98.722 | 41.207 | 1.00 | 26.69 | 6 |
| 5078 | CE | LYS A 654 | 18.152 | 94.544 | 42.680 | 1.00 | 30.47 | 6 | 5120 | CG1 | ILE A 660 | 13.012 | 97.534 | 41.991 | 1.00 | 27.58 | 6 |
| 5079 | NZ | LYS A 654 | 17.967 | 93.152 | 43.221 | 1.00 | 39.55 | 7 | 5121 | CG2 | ILE A 660 | 11.704 | 98.273 | 39.972 | 1.00 | 21.18 | 6 |
| 5080 | N | ARG A 655 | 18.538 | 99.361 | 39.337 | 1.00 | 19.37 | 7 | 5122 | CD1 | ILE A 660 | 14.022 | 96.722 | 41.221 | 1.00 | 24.46 | 6 |
| 5081 | CA | ARG A 655 | 19.776 | 100.164 | 39.391 | 1.00 | 21.00 | 6 | 5123 | N | GLN A 661 | 13.169 | 100.849 | 38.624 | 1.00 | 20.86 | 7 |
| 5082 | C | ARG A 655 | 20.820 | 99.478 | 40.256 | 1.00 | 24.58 | 6 | 5124 | CA | GLN A 661 | 12.479 | 101.793 | 37.743 | 1.00 | 19.49 | 6 |
| 5083 | O | ARG A 655 | 20.486 | 98.604 | 41.057 | 1.00 | 22.97 | 8 | 5125 | C | GLN A 661 | 11.720 | 101.014 | 36.669 | 1.00 | 20.02 | 6 |
| 5084 | CB | ARG A 655 | 19.445 | 101.531 | 40.003 | 1.00 | 18.71 | 6 | 5126 | O | GLN A 661 | 12.266 | 100.405 | 35.730 | 1.00 | 19.24 | 8 |
| 5085 | CG | ARG A 655 | 18.411 | 102.323 | 39.192 | 1.00 | 19.26 | 6 | 5127 | CB | GLN A 661 | 13.410 | 102.775 | 37.023 | 1.00 | 20.06 | 6 |
| 5086 | CD | ARG A 655 | 19.036 | 102.699 | 37.864 | 1.00 | 24.72 | 6 | 5128 | CG | GLN A 661 | 12.611 | 103.688 | 36.077 | 1.00 | 21.00 | 6 |
| 5087 | NE | ARG A 655 | 18.169 | 103.597 | 37.102 | 1.00 | 23.26 | 7 | 5129 | CD | GLN A 661 | 13.541 | 104.665 | 35.350 | 1.00 | 21.47 | 6 |
| 5088 | CZ | ARG A 655 | 18.428 | 104.073 | 35.883 | 1.00 | 23.74 | 6 | 5130 | OE1 | GLN A 661 | 13.279 | 104.997 | 34.195 | 1.00 | 28.51 | 8 |
| 5089 | NH1 | ARG A 655 | 19.508 | 103.812 | 35.193 | 1.00 | 20.63 | 7 | 5131 | NE2 | GLN A 661 | 14.578 | 105.095 | 36.040 | 1.00 | 22.67 | 7 |
| 5090 | NH2 | ARG A 655 | 17.509 | 104.882 | 35.343 | 1.00 | 24.30 | 7 | 5132 | N | TRP A 662 | 10.389 | 100.926 | 36.834 | 1.00 | 20.75 | 7 |
| 5091 | N | ALA A 656 | 22.090 | 99.900 | 40.135 | 1.00 | 24.51 | 7 | 5133 | CA | TRP A 662 | 9.556 | 100.227 | 35.857 | 1.00 | 18.49 | 6 |
| 5092 | CA | ALA A 656 | 23.170 | 99.305 | 40.898 | 1.00 | 28.24 | 6 | 5134 | C | TRP A 662 | 9.441 | 100.967 | 34.536 | 1.00 | 21.67 | 6 |
| 5093 | C | ALA A 656 | 22.865 | 99.430 | 42.401 | 1.00 | 27.25 | 6 | 5135 | O | TRP A 662 | 9.412 | 102.230 | 34.565 | 1.00 | 19.29 | 8 |
| 5094 | O | ALA A 656 | 23.305 | 98.533 | 43.117 | 1.00 | 32.90 | 8 | 5136 | CB | TRP A 662 | 8.152 | 100.082 | 36.437 | 1.00 | 18.81 | 6 |
| 5095 | CB | ALA A 656 | 24.518 | 100.009 | 40.656 | 1.00 | 29.09 | 6 | 5137 | CG | TRP A 662 | 7.960 | 99.114 | 37.551 | 1.00 | 18.39 | 6 |
| 5096 | N | ASP A 657 | 22.145 | 100.427 | 42.856 | 1.00 | 31.34 | 7 | 5138 | CD1 | TRP A 662 | 8.083 | 99.359 | 38.889 | 1.00 | 19.35 | 6 |
| 5097 | CA | ASP A 657 | 21.850 | 100.561 | 44.282 | 1.00 | 32.95 | 6 | 5139 | CD2 | TRP A 662 | 7.543 | 97.752 | 37.419 | 1.00 | 18.13 | 6 |

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|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| 5140 | NE1 | TRP | A | 662 | 7.781 | 98.218 | 39.608 | 1.00 | 21.46 | 7 | 5182 | CA | HIS | A | 668 | 2.882 | 94.747 | 26.930 | 1.00 | 15.66 | 6 |
| 5141 | CE2 | TRP | A | 662 | 7.444 | 97.223 | 38.713 | 1.00 | 18.92 | 6 | 5183 | C | HIS | A | 668 | 2.137 | 93.408 | 26.856 | 1.00 | 16.10 | 6 |
| 5142 | CE3 | TRP | A | 662 | 7.213 | 96.960 | 36.295 | 1.00 | 18.78 | 6 | 5184 | O | HIS | A | 668 | 2.048 | 92.666 | 27.847 | 1.00 | 16.87 | 8 |
| 5143 | C22 | TRP | A | 662 | 6.994 | 95.923 | 38.966 | 1.00 | 16.39 | 6 | 5185 | CB | HIS | A | 668 | 4.327 | 94.431 | 26.491 | 1.00 | 15.51 | 6 |
| 5144 | C23 | TRP | A | 662 | 6.798 | 95.661 | 36.537 | 1.00 | 18.67 | 6 | 5186 | CG | HIS | A | 668 | 5.208 | 95.653 | 26.519 | 1.00 | 14.13 | 6 |
| 5145 | CH2 | TRP | A | 662 | 6.725 | 95.156 | 37.854 | 1.00 | 15.44 | 6 | 5187 | ND1 | HIS | A | 668 | 5.229 | 96.451 | 25.375 | 1.00 | 15.75 | 7 |
| 5146 | N | GLU | A | 663 | 9.170 | 100.250 | 33.453 | 1.00 | 18.24 | 7 | 5188 | CD2 | HIS | A | 668 | 6.066 | 96.158 | 27.410 | 1.00 | 17.00 | 6 |
| 5147 | CA | GLU | A | 663 | 8.551 | 100.857 | 32.292 | 1.00 | 17.79 | 6 | 5189 | CE1 | HIS | A | 668 | 6.108 | 97.464 | 25.592 | 1.00 | 14.21 | 6 |
| 5148 | C | GLU | A | 663 | 7.240 | 101.517 | 32.740 | 1.00 | 17.95 | 6 | 5190 | NE2 | HIS | A | 668 | 6.581 | 97.305 | 26.830 | 1.00 | 15.51 | 7 |
| 5149 | O | GLU | A | 663 | 6.519 | 100.973 | 33.574 | 1.00 | 18.49 | 8 | 5191 | N | VAL | A | 669 | 1.434 | 93.208 | 25.734 | 1.00 | 15.02 | 7 |
| 5150 | CB | GLU | A | 663 | 8.001 | 99.880 | 31.232 | 1.00 | 22.54 | 6 | 5192 | CA | VAL | A | 669 | 0.684 | 91.987 | 25.490 | 1.00 | 16.94 | 6 |
| 5151 | CG | GLU | A | 663 | 9.065 | 99.526 | 30.195 | 1.00 | 23.03 | 6 | 5193 | C | VAL | A | 669 | 1.205 | 91.294 | 24.260 | 1.00 | 14.25 | 6 |
| 5152 | CD | GLU | A | 663 | 8.380 | 98.560 | 29.223 | 1.00 | 19.52 | 6 | 5194 | O | VAL | A | 669 | 1.414 | 91.936 | 23.206 | 1.00 | 17.08 | 8 |
| 5153 | OE1 | GLU | A | 663 | 8.159 | 97.397 | 29.619 | 1.00 | 17.12 | 8 | 5195 | CB | VAL | A | 669 | -0.852 | 92.295 | 25.322 | 1.00 | 17.60 | 6 |
| 5154 | OE2 | GLU | A | 663 | 8.063 | 98.990 | 28.102 | 1.00 | 18.01 | 8 | 5196 | CG1 | VAL | A | 669 | -1.624 | 90.970 | 25.253 | 1.00 | 20.63 | 6 |
| 5155 | N | ASN | A | 664 | 6.892 | 102.576 | 32.027 | 1.00 | 18.62 | 7 | 5197 | CG2 | VAL | A | 669 | -1.341 | 93.078 | 26.547 | 1.00 | 17.53 | 6 |
| 5156 | CA | ASN | A | 664 | 5.604 | 103.189 | 32.365 | 1.00 | 18.27 | 6 | 5198 | N | ALA | A | 670 | 1.450 | 89.971 | 24.287 | 1.00 | 14.50 | 7 |
| 5157 | C | ASN | A | 664 | 4.522 | 102.581 | 31.484 | 1.00 | 20.85 | 6 | 5199 | CA | ALA | A | 670 | 1.945 | 89.249 | 23.113 | 1.00 | 14.21 | 6 |
| 5158 | O | ASN | A | 664 | 4.782 | 101.671 | 30.702 | 1.00 | 21.34 | 8 | 5200 | C | ALA | A | 670 | 1.437 | 87.798 | 23.234 | 1.00 | 15.38 | 6 |
| 5159 | CB | ASN | A | 664 | 5.790 | 104.696 | 32.115 | 1.00 | 22.20 | 6 | 5201 | O | ALA | A | 670 | 1.216 | 87.262 | 24.323 | 1.00 | 15.04 | 8 |
| 5160 | CG | ASN | A | 664 | 6.447 | 105.326 | 33.350 | 1.00 | 30.00 | 6 | 5202 | CB | ALA | A | 670 | 3.481 | 89.251 | 23.005 | 1.00 | 14.71 | 6 |
| 5161 | OD1 | ASN | A | 664 | 6.281 | 104.932 | 34.519 | 1.00 | 35.11 | 8 | 5203 | N | THR | A | 671 | 1.412 | 87.143 | 22.093 | 1.00 | 15.66 | 7 |
| 5162 | ND2 | ASN | A | 664 | 7.238 | 106.366 | 33.127 | 1.00 | 33.46 | 7 | 5204 | CA | THR | A | 671 | 1.145 | 85.704 | 22.056 | 1.00 | 15.06 | 6 |
| 5163 | N | GLY | A | 665 | 3.295 | 103.085 | 31.667 | 1.00 | 22.07 | 7 | 5205 | C | THR | A | 671 | 2.463 | 85.017 | 21.737 | 1.00 | 15.13 | 6 |
| 5164 | CA | GLY | A | 665 | 2.187 | 102.708 | 30.786 | 1.00 | 23.10 | 6 | 5206 | O | THR | A | 671 | 3.141 | 85.293 | 20.734 | 1.00 | 16.78 | 8 |
| 5165 | C | GLY | A | 665 | 1.557 | 101.363 | 31.102 | 1.00 | 21.34 | 6 | 5207 | CB | THR | A | 671 | 0.004 | 85.374 | 21.082 | 1.00 | 24.32 | 6 |
| 5166 | O | GLY | A | 665 | 1.827 | 100.710 | 32.119 | 1.00 | 22.70 | 8 | 5208 | CG1 | THR | A | 671 | -1.181 | 86.041 | 21.584 | 1.00 | 19.33 | 8 |
| 5167 | N | SER | A | 666 | 0.832 | 100.839 | 30.093 | 1.00 | 18.43 | 7 | 5209 | CG2 | THR | A | 671 | -0.323 | 83.900 | 21.063 | 1.00 | 22.47 | 6 |
| 5168 | CA | SER | A | 666 | 0.135 | 99.581 | 30.305 | 1.00 | 17.79 | 6 | 5210 | N | THR | A | 672 | 2.794 | 83.967 | 22.533 | 1.00 | 13.36 | 7 |
| 5169 | C | SER | A | 666 | 1.084 | 98.403 | 30.046 | 1.00 | 16.94 | 6 | 5211 | CA | THR | A | 672 | 4.035 | 83.264 | 22.249 | 1.00 | 14.54 | 6 |
| 5170 | O | SER | A | 666 | 2.005 | 98.503 | 29.261 | 1.00 | 16.68 | 8 | 5212 | C | THR | A | 672 | 3.911 | 82.312 | 21.096 | 1.00 | 14.80 | 6 |
| 5171 | CB | SER | A | 666 | -1.037 | 99.440 | 29.297 | 1.00 | 24.19 | 6 | 5213 | O | THR | A | 672 | 2.831 | 81.798 | 20.772 | 1.00 | 13.92 | 8 |
| 5172 | OG | SER | A | 666 | -1.959 | 100.498 | 29.645 | 1.00 | 24.86 | 8 | 5214 | CB | THR | A | 672 | 4.475 | 82.464 | 23.491 | 1.00 | 15.06 | 6 |
| 5173 | N | ASN | A | 667 | 0.642 | 97.227 | 30.470 | 1.00 | 14.27 | 7 | 5215 | OG1 | THR | A | 672 | 3.485 | 81.497 | 23.805 | 1.00 | 13.92 | 8 |
| 5174 | CA | ASN | A | 667 | 1.491 | 96.058 | 30.168 | 1.00 | 16.75 | 6 | 5216 | CG2 | THR | A | 672 | 4.612 | 83.376 | 24.726 | 1.00 | 15.62 | 6 |
| 5175 | C | ASN | A | 667 | 1.575 | 95.824 | 28.678 | 1.00 | 17.00 | 6 | 5217 | N | PRO | A | 673 | 5.068 | 81.983 | 20.499 | 1.00 | 16.20 | 7 |
| 5176 | O | ASN | A | 667 | 0.616 | 96.050 | 27.899 | 1.00 | 15.91 | 8 | 5218 | CA | PRO | A | 673 | 5.116 | 81.063 | 19.381 | 1.00 | 21.02 | 6 |
| 5177 | CB | ASN | A | 667 | 0.795 | 94.804 | 30.736 | 1.00 | 16.66 | 6 | 5219 | C | PRO | A | 673 | 4.615 | 79.690 | 19.691 | 1.00 | 17.09 | 6 |
| 5178 | CG | ASN | A | 667 | 0.703 | 94.817 | 32.248 | 1.00 | 19.33 | 6 | 5220 | O | PRO | A | 673 | 4.691 | 79.290 | 20.893 | 1.00 | 16.99 | 8 |
| 5179 | OD1 | ASN | A | 667 | -0.178 | 94.105 | 32.855 | 1.00 | 20.96 | 8 | 5221 | CB | PRO | A | 673 | 6.606 | 80.975 | 18.937 | 1.00 | 22.47 | 6 |
| 5180 | ND2 | ASN | A | 667 | 1.594 | 95.513 | 32.887 | 1.00 | 16.21 | 7 | 5222 | CG | PRO | A | 673 | 7.309 | 81.859 | 19.872 | 1.00 | 22.50 | 6 |
| 5181 | N | HIS | A | 668 | 2.720 | 95.243 | 28.272 | 1.00 | 13.63 | 7 | 5223 | CD | PRO | A | 673 | 6.355 | 82.558 | 20.857 | 1.00 | 20.76 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|---|------|-----|-----------|--------|---------|--------|------|-------|---|
| 5224 | N | THR A 674 | 4.164 | 78.885 | 18.724 | 1.00 | 16.36 | 7 | 5266 | CD1 | ILE A 680 | 6.611 | 86.867 | 23.218 | 1.00 | 15.15 | 6 |
| 5225 | CA | THR A 674 | 3.803 | 77.518 | 19.033 | 1.00 | 16.04 | 6 | 5267 | N | THR A 681 | 9.363 | 91.378 | 20.334 | 1.00 | 13.57 | 7 |
| 5226 | C | THR A 674 | 4.915 | 76.516 | 18.803 | 1.00 | 19.50 | 6 | 5268 | CA | THR A 681 | 10.236 | 92.583 | 20.392 | 1.00 | 12.91 | 6 |
| 5227 | O | THR A 674 | 4.834 | 75.399 | 19.293 | 1.00 | 25.45 | 8 | 5269 | C | THR A 681 | 9.280 | 93.751 | 20.616 | 1.00 | 13.01 | 6 |
| 5228 | CB | THR A 674 | 2.613 | 77.053 | 18.117 | 1.00 | 26.38 | 6 | 5270 | O | THR A 681 | 8.253 | 93.845 | 19.929 | 1.00 | 18.59 | 8 |
| 5229 | CG1 | THR A 674 | 2.997 | 77.353 | 16.786 | 1.00 | 31.27 | 8 | 5271 | CB | THR A 681 | 10.904 | 92.718 | 18.990 | 1.00 | 16.97 | 6 |
| 5230 | CG2 | THR A 674 | 1.409 | 77.936 | 18.521 | 1.00 | 27.63 | 6 | 5272 | OG1 | THR A 681 | 11.807 | 91.633 | 18.765 | 1.00 | 17.30 | 8 |
| 5231 | N | GLY A 675 | 5.953 | 76.981 | 18.114 | 1.00 | 19.68 | 7 | 5273 | CG2 | THR A 681 | 11.642 | 94.052 | 18.964 | 1.00 | 19.53 | 6 |
| 5232 | CA | GLY A 675 | 7.035 | 76.041 | 17.829 | 1.00 | 18.98 | 6 | 5274 | N | VAL A 682 | 9.639 | 94.595 | 21.608 | 1.00 | 15.51 | 7 |
| 5233 | C | GLY A 675 | 8.164 | 76.145 | 18.885 | 1.00 | 21.20 | 6 | 5275 | CA | VAL A 682 | 8.758 | 95.732 | 21.946 | 1.00 | 15.78 | 6 |
| 5234 | N | GLY A 675 | 7.915 | 76.654 | 19.953 | 1.00 | 18.10 | 8 | 5276 | C | VAL A 682 | 9.635 | 96.952 | 22.186 | 1.00 | 17.87 | 6 |
| 5235 | O | ALA A 676 | 9.349 | 75.612 | 18.560 | 1.00 | 14.92 | 7 | 5277 | O | VAL A 682 | 10.838 | 96.797 | 22.256 | 1.00 | 15.49 | 8 |
| 5236 | CA | ALA A 676 | 10.419 | 75.562 | 19.578 | 1.00 | 12.67 | 6 | 5278 | CB | VAL A 682 | 7.874 | 95.472 | 23.195 | 1.00 | 16.15 | 6 |
| 5237 | C | ALA A 676 | 10.845 | 76.968 | 19.974 | 1.00 | 13.87 | 6 | 5279 | CG1 | VAL A 682 | 6.968 | 94.243 | 23.002 | 1.00 | 16.76 | 6 |
| 5238 | O | ALA A 676 | 11.505 | 77.096 | 21.031 | 1.00 | 12.93 | 8 | 5280 | CG2 | VAL A 682 | 8.730 | 95.365 | 24.469 | 1.00 | 16.17 | 6 |
| 5239 | CB | ALA A 676 | 11.611 | 74.771 | 19.006 | 1.00 | 12.85 | 6 | 5281 | N | THR A 683 | 9.082 | 98.162 | 22.306 | 1.00 | 15.89 | 7 |
| 5240 | N | THR A 677 | 10.860 | 77.884 | 19.014 | 1.00 | 13.69 | 7 | 5282 | CA | THR A 683 | 9.863 | 99.346 | 22.623 | 1.00 | 15.51 | 6 |
| 5241 | CA | THR A 677 | 11.444 | 79.189 | 19.324 | 1.00 | 11.81 | 6 | 5283 | C | THR A 683 | 9.529 | 99.798 | 22.046 | 1.00 | 16.36 | 6 |
| 5242 | C | THR A 677 | 10.615 | 80.296 | 18.686 | 1.00 | 13.20 | 6 | 5284 | O | THR A 683 | 8.371 | 99.703 | 24.462 | 1.00 | 17.59 | 8 |
| 5243 | O | THR A 677 | 9.743 | 80.066 | 17.834 | 1.00 | 14.64 | 8 | 5285 | CB | THR A 683 | 9.481 | 100.473 | 21.614 | 1.00 | 22.31 | 6 |
| 5244 | CB | THR A 677 | 12.847 | 79.366 | 18.681 | 1.00 | 14.32 | 6 | 5286 | OG1 | THR A 683 | 9.916 | 100.019 | 20.328 | 1.00 | 21.22 | 8 |
| 5245 | OG1 | THR A 677 | 12.712 | 79.294 | 17.249 | 1.00 | 16.35 | 8 | 5287 | CG2 | THR A 683 | 10.245 | 101.759 | 21.921 | 1.00 | 19.31 | 6 |
| 5246 | CG2 | THR A 677 | 13.851 | 78.287 | 19.079 | 1.00 | 14.03 | 6 | 5288 | N | TRP A 684 | 10.586 | 100.168 | 24.759 | 1.00 | 14.24 | 7 |
| 5247 | N | GLY A 678 | 10.949 | 81.490 | 19.141 | 1.00 | 14.25 | 7 | 5289 | CA | TRP A 684 | 10.411 | 100.587 | 26.154 | 1.00 | 14.76 | 6 |
| 5248 | CA | GLY A 678 | 10.413 | 82.685 | 18.437 | 1.00 | 13.38 | 6 | 5290 | C | TRP A 684 | 9.369 | 101.706 | 26.222 | 1.00 | 17.75 | 6 |
| 5249 | C | GLY A 678 | 10.969 | 83.958 | 19.066 | 1.00 | 13.68 | 6 | 5291 | O | TRP A 684 | 9.556 | 102.695 | 25.469 | 1.00 | 18.74 | 8 |
| 5250 | O | GLY A 678 | 11.857 | 83.956 | 19.907 | 1.00 | 13.62 | 8 | 5292 | CB | TRP A 684 | 11.745 | 101.086 | 26.705 | 1.00 | 14.95 | 6 |
| 5251 | N | ASN A 679 | 10.374 | 85.094 | 18.654 | 1.00 | 13.18 | 7 | 5293 | CG | TRP A 684 | 11.696 | 101.465 | 28.146 | 1.00 | 14.49 | 6 |
| 5252 | CA | ASN A 679 | 10.858 | 86.398 | 19.082 | 1.00 | 11.86 | 6 | 5294 | CD1 | TRP A 684 | 11.284 | 102.666 | 28.672 | 1.00 | 15.39 | 6 |
| 5253 | C | ASN A 679 | 9.685 | 87.318 | 19.466 | 1.00 | 14.28 | 6 | 5295 | CD2 | TRP A 684 | 12.163 | 100.683 | 29.271 | 1.00 | 17.84 | 6 |
| 5254 | O | ASN A 679 | 8.718 | 87.315 | 18.699 | 1.00 | 15.54 | 8 | 5296 | NE1 | TRP A 684 | 11.376 | 102.649 | 30.052 | 1.00 | 16.11 | 7 |
| 5255 | CB | ASN A 679 | 11.485 | 87.180 | 17.892 | 1.00 | 16.45 | 6 | 5297 | CE2 | TRP A 684 | 11.921 | 101.440 | 30.423 | 1.00 | 20.66 | 6 |
| 5256 | CG | ASN A 679 | 12.952 | 86.818 | 17.758 | 1.00 | 25.76 | 6 | 5298 | CE3 | TRP A 684 | 12.764 | 99.422 | 29.399 | 1.00 | 18.28 | 6 |
| 5257 | OD1 | ASN A 679 | 13.201 | 85.708 | 17.294 | 1.00 | 24.19 | 8 | 5299 | C22 | TRP A 684 | 12.245 | 101.024 | 31.726 | 1.00 | 22.23 | 6 |
| 5258 | ND2 | ASN A 679 | 13.881 | 87.684 | 18.146 | 1.00 | 26.44 | 7 | 5300 | C23 | TRP A 684 | 13.074 | 98.959 | 30.709 | 1.00 | 17.05 | 6 |
| 5259 | N | ILE A 680 | 9.882 | 88.063 | 20.521 | 1.00 | 13.28 | 7 | 5301 | CH2 | TRP A 684 | 12.791 | 99.766 | 31.796 | 1.00 | 17.97 | 6 |
| 5260 | CA | ILE A 680 | 8.909 | 89.088 | 20.948 | 1.00 | 14.10 | 6 | 5302 | N | GLN A 685 | 8.396 | 101.650 | 27.102 | 1.00 | 17.70 | 7 |
| 5261 | C | ILE A 680 | 9.758 | 90.331 | 21.093 | 1.00 | 16.54 | 6 | 5303 | CA | GLN A 685 | 7.399 | 102.716 | 27.315 | 1.00 | 18.97 | 6 |
| 5262 | O | ILE A 680 | 10.673 | 90.366 | 21.944 | 1.00 | 14.10 | 8 | 5304 | C | GLN A 685 | 7.850 | 103.719 | 28.333 | 1.00 | 19.08 | 6 |
| 5263 | CB | ILE A 680 | 8.224 | 88.676 | 22.277 | 1.00 | 13.96 | 6 | 5305 | O | GLN A 685 | 8.067 | 103.430 | 29.512 | 1.00 | 19.01 | 8 |
| 5264 | CG1 | ILE A 680 | 7.245 | 87.519 | 21.978 | 1.00 | 16.92 | 6 | 5306 | CB | GLN A 685 | 6.071 | 102.025 | 27.745 | 1.00 | 15.69 | 6 |
| 5265 | CG2 | ILE A 680 | 7.442 | 89.919 | 22.790 | 1.00 | 17.42 | 6 | 5307 | CG | GLN A 685 | 5.536 | 101.157 | 26.596 | 1.00 | 17.89 | 6 |

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|------|-----|-----------|--------|---------|--------|------|-------|---|------|-----|-----------|--------|--------|--------|------|-------|---|
| 5308 | CD | GLN A 685 | 4.352 | 100.283 | 26.995 | 1.00 | 18.78 | 6 | 5350 | C36 | HEX A 690 | 37.084 | 73.167 | 28.829 | 1.00 | 13.71 | 6 |
| 5309 | OE1 | GLN A 685 | 3.797 | 99.604 | 26.110 | 1.00 | 20.58 | 8 | 5351 | C41 | HEX A 690 | 33.322 | 71.601 | 28.292 | 1.00 | 9.18 | 6 |
| 5310 | NE2 | GLN A 685 | 3.960 | 100.246 | 28.267 | 1.00 | 17.75 | 7 | 5352 | N41 | HEX A 690 | 34.214 | 72.300 | 29.267 | 1.00 | 10.73 | 7 |
| 5311 | N | ASN A 686 | 8.037 | 105.011 | 27.906 | 1.00 | 21.27 | 7 | 5353 | C42 | HEX A 690 | 33.682 | 70.074 | 28.156 | 1.00 | 11.48 | 6 |
| 5312 | CA | ASN A 686 | 8.547 | 106.008 | 28.836 | 1.00 | 20.38 | 6 | 5354 | O42 | HEX A 690 | 33.732 | 69.433 | 29.448 | 1.00 | 10.30 | 8 |
| 5313 | C | ASN A 686 | 7.489 | 106.854 | 29.654 | 1.00 | 22.87 | 6 | 5355 | C43 | HEX A 690 | 35.023 | 69.963 | 27.455 | 1.00 | 10.39 | 6 |
| 5314 | O | ASN A 686 | 6.387 | 106.692 | 29.016 | 1.00 | 22.87 | 8 | 5356 | O43 | HEX A 690 | 35.686 | 68.699 | 27.591 | 1.00 | 11.44 | 8 |
| 5315 | CB | ASN A 686 | 9.300 | 107.060 | 27.975 | 1.00 | 24.12 | 6 | 5357 | C44 | HEX A 690 | 34.791 | 70.257 | 25.986 | 1.00 | 11.02 | 6 |
| 5316 | CG | ASN A 686 | 10.434 | 106.404 | 27.176 | 1.00 | 23.38 | 6 | 5358 | C45 | HEX A 690 | 33.925 | 71.520 | 25.899 | 1.00 | 10.58 | 6 |
| 5317 | OD1 | ASN A 686 | 11.360 | 105.896 | 27.821 | 1.00 | 22.76 | 8 | 5359 | C40 | HEX A 690 | 33.262 | 72.097 | 26.944 | 1.00 | 9.08 | 6 |
| 5318 | ND2 | ASN A 686 | 10.376 | 106.412 | 25.832 | 1.00 | 25.47 | 7 | 5360 | C46 | HEX A 690 | 33.519 | 71.887 | 24.466 | 1.00 | 12.28 | 6 |
| 5319 | C11 | HEX A 690 | 38.644 | 78.012 | 38.228 | 1.00 | 27.46 | 6 | 5361 | O46 | HEX A 690 | 32.492 | 71.022 | 24.020 | 1.00 | 12.58 | 8 |
| 5320 | O11 | HEX A 690 | 39.147 | 78.243 | 39.503 | 1.00 | 37.24 | 8 | 5362 | C51 | HEX A 690 | 36.288 | 69.864 | 24.116 | 1.00 | 10.88 | 6 |
| 5321 | C12 | HEX A 690 | 37.596 | 79.172 | 38.058 | 1.00 | 23.95 | 6 | 5363 | O51 | HEX A 690 | 36.061 | 70.541 | 25.327 | 1.00 | 12.10 | 8 |
| 5322 | O12 | HEX A 690 | 36.681 | 78.887 | 39.109 | 1.00 | 20.96 | 8 | 5364 | C52 | HEX A 690 | 37.495 | 68.906 | 24.274 | 1.00 | 11.69 | 6 |
| 5323 | C13 | HEX A 690 | 36.915 | 78.887 | 36.685 | 1.00 | 17.64 | 6 | 5365 | O52 | HEX A 690 | 37.227 | 67.917 | 25.285 | 1.00 | 12.57 | 8 |
| 5324 | O13 | HEX A 690 | 35.915 | 79.908 | 36.442 | 1.00 | 18.04 | 8 | 5366 | C53 | HEX A 690 | 38.717 | 69.698 | 24.774 | 1.00 | 10.51 | 6 |
| 5325 | C14 | HEX A 690 | 38.048 | 79.023 | 35.670 | 1.00 | 17.74 | 6 | 5367 | O53 | HEX A 690 | 39.832 | 68.756 | 24.609 | 1.00 | 11.97 | 8 |
| 5326 | O15 | HEX A 690 | 39.141 | 77.967 | 35.956 | 1.00 | 19.52 | 6 | 5368 | C54 | HEX A 690 | 39.025 | 70.807 | 23.714 | 1.00 | 12.82 | 6 |
| 5327 | C15 | HEX A 690 | 39.679 | 78.312 | 37.276 | 1.00 | 26.20 | 8 | 5369 | C55 | HEX A 690 | 37.748 | 71.660 | 23.566 | 1.00 | 12.56 | 6 |
| 5328 | C16 | HEX A 690 | 40.338 | 77.919 | 35.016 | 1.00 | 23.71 | 6 | 5370 | O55 | HEX A 690 | 36.680 | 70.820 | 23.133 | 1.00 | 11.57 | 8 |
| 5329 | O16 | HEX A 690 | 40.867 | 79.240 | 34.817 | 1.00 | 28.38 | 8 | 5371 | C56 | HEX A 690 | 37.890 | 72.687 | 22.436 | 1.00 | 12.61 | 6 |
| 5330 | C21 | HEX A 690 | 37.609 | 79.324 | 33.250 | 1.00 | 19.03 | 6 | 5372 | O56 | HEX A 690 | 38.082 | 72.074 | 21.134 | 1.00 | 19.74 | 8 |
| 5331 | O21 | HEX A 690 | 37.414 | 78.562 | 34.414 | 1.00 | 18.39 | 8 | 5373 | C61 | HEX A 690 | 40.720 | 72.590 | 24.188 | 1.00 | 22.95 | 6 |
| 5332 | C22 | HEX A 690 | 36.237 | 79.756 | 32.692 | 1.00 | 18.97 | 6 | 5374 | O61 | HEX A 690 | 39.890 | 71.572 | 24.637 | 1.00 | 20.26 | 8 |
| 5333 | O22 | HEX A 690 | 35.419 | 80.404 | 33.669 | 1.00 | 17.96 | 8 | 5375 | C62 | HEX A 690 | 42.050 | 72.500 | 24.991 | 1.00 | 23.13 | 6 |
| 5334 | C23 | HEX A 690 | 35.514 | 78.516 | 32.153 | 1.00 | 16.72 | 6 | 5376 | O62 | HEX A 690 | 42.582 | 71.189 | 24.918 | 1.00 | 23.06 | 8 |
| 5335 | O23 | HEX A 690 | 34.355 | 79.014 | 31.406 | 1.00 | 16.31 | 8 | 5377 | C63 | HEX A 690 | 41.937 | 73.006 | 26.411 | 1.00 | 24.03 | 6 |
| 5336 | C24 | HEX A 690 | 36.415 | 77.760 | 31.174 | 1.00 | 12.77 | 6 | 5378 | O63 | HEX A 690 | 43.280 | 72.994 | 26.932 | 1.00 | 28.78 | 8 |
| 5337 | C25 | HEX A 690 | 37.690 | 77.301 | 31.955 | 1.00 | 17.32 | 6 | 5379 | C64 | HEX A 690 | 41.310 | 74.405 | 26.428 | 1.00 | 25.79 | 6 |
| 5338 | O25 | HEX A 690 | 38.321 | 78.596 | 32.286 | 1.00 | 20.72 | 8 | 5380 | O64 | HEX A 690 | 41.035 | 74.789 | 27.809 | 1.00 | 29.96 | 8 |
| 5339 | C26 | HEX A 690 | 38.704 | 76.681 | 30.979 | 1.00 | 18.94 | 6 | 5381 | C65 | HEX A 690 | 39.918 | 74.255 | 25.759 | 1.00 | 22.19 | 6 |
| 5340 | O26 | HEX A 690 | 39.852 | 76.182 | 31.780 | 1.00 | 21.07 | 8 | 5382 | O65 | HEX A 690 | 40.146 | 73.866 | 24.404 | 1.00 | 22.47 | 8 |
| 5341 | C31 | HEX A 690 | 35.507 | 76.403 | 29.409 | 1.00 | 11.28 | 6 | 5383 | C66 | HEX A 690 | 39.177 | 75.555 | 25.611 | 1.00 | 26.12 | 6 |
| 5342 | O31 | HEX A 690 | 35.723 | 76.501 | 30.811 | 1.00 | 12.85 | 8 | 5384 | O66 | HEX A 690 | 39.936 | 76.644 | 25.149 | 1.00 | 24.41 | 8 |
| 5343 | C32 | HEX A 690 | 34.026 | 76.118 | 29.118 | 1.00 | 13.04 | 6 | 5385 | C11 | MAL A 691 | 38.534 | 71.299 | 69.464 | 1.00 | 19.75 | 6 |
| 5344 | O32 | HEX A 690 | 33.259 | 77.030 | 29.933 | 1.00 | 14.06 | 8 | 5386 | O11 | MAL A 691 | 38.776 | 72.581 | 69.883 | 1.00 | 20.21 | 8 |
| 5345 | C33 | HEX A 690 | 33.654 | 74.698 | 29.626 | 1.00 | 13.59 | 6 | 5387 | C12 | MAL A 691 | 37.973 | 71.384 | 68.024 | 1.00 | 17.66 | 6 |
| 5346 | O33 | HEX A 690 | 32.285 | 74.486 | 29.158 | 1.00 | 12.48 | 8 | 5388 | O12 | MAL A 691 | 38.798 | 72.262 | 67.225 | 1.00 | 18.71 | 8 |
| 5347 | C34 | HEX A 690 | 34.578 | 73.670 | 28.936 | 1.00 | 11.83 | 6 | 5389 | C13 | MAL A 691 | 36.555 | 71.949 | 68.006 | 1.00 | 16.03 | 6 |
| 5348 | C35 | HEX A 690 | 36.004 | 74.036 | 29.487 | 1.00 | 14.01 | 6 | 5390 | O13 | MAL A 691 | 35.969 | 71.754 | 66.689 | 1.00 | 17.47 | 8 |
| 5349 | O35 | HEX A 690 | 36.301 | 75.341 | 28.930 | 1.00 | 12.70 | 8 | 5391 | C14 | MAL A 691 | 35.642 | 71.104 | 68.925 | 1.00 | 15.64 | 6 |

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|------|-----|-----------|--------|--------|--------|------|-------|----|------|-----|-------|----|--------|--------|--------|------|-------|---|
| 5392 | C15 | MAL A 691 | 36.269 | 71.291 | 70.364 | 1.00 | 14.01 | 6 | 5472 | OWO | WAT V | 19 | 26.088 | 62.658 | 22.854 | 1.00 | 11.54 | 8 |
| 5393 | O15 | MAL A 691 | 37.561 | 70.667 | 70.312 | 1.00 | 16.48 | 8 | 5473 | OWO | WAT V | 20 | 37.981 | 63.919 | 14.127 | 1.00 | 11.77 | 8 |
| 5394 | C16 | MAL A 691 | 35.519 | 70.221 | 71.238 | 1.00 | 19.77 | 6 | 5474 | OWO | WAT V | 21 | 34.932 | 60.656 | 13.769 | 1.00 | 11.70 | 8 |
| 5395 | O16 | MAL A 691 | 36.004 | 70.431 | 72.581 | 1.00 | 18.54 | 8 | 5475 | OWO | WAT V | 22 | 41.499 | 60.656 | 38.722 | 1.00 | 11.54 | 8 |
| 5396 | C21 | MAL A 691 | 33.285 | 70.813 | 68.523 | 1.00 | 18.83 | 6 | 5476 | OWO | WAT V | 23 | 40.945 | 66.711 | 20.205 | 1.00 | 11.65 | 8 |
| 5397 | O21 | MAL A 691 | 34.336 | 71.683 | 68.968 | 1.00 | 17.92 | 8 | 5477 | OWO | WAT V | 24 | 8.905 | 64.107 | 34.370 | 1.00 | 11.68 | 8 |
| 5398 | C22 | MAL A 691 | 32.403 | 71.638 | 67.561 | 1.00 | 17.24 | 6 | 5478 | OWO | WAT V | 25 | 19.426 | 72.356 | 40.893 | 1.00 | 11.74 | 8 |
| 5399 | O22 | MAL A 691 | 33.177 | 72.083 | 66.433 | 1.00 | 17.89 | 8 | 5479 | OWO | WAT V | 26 | 20.321 | 82.331 | 35.376 | 1.00 | 11.77 | 8 |
| 5400 | C23 | MAL A 691 | 31.765 | 72.820 | 68.304 | 1.00 | 18.41 | 6 | 5480 | OWO | WAT V | 27 | 14.993 | 64.250 | 37.502 | 1.00 | 11.91 | 8 |
| 5401 | O23 | MAL A 691 | 30.812 | 73.419 | 67.431 | 1.00 | 18.30 | 8 | 5481 | OWO | WAT V | 28 | 31.504 | 68.673 | 10.842 | 1.00 | 12.08 | 8 |
| 5402 | C24 | MAL A 691 | 30.951 | 72.194 | 69.478 | 1.00 | 18.57 | 6 | 5482 | OWO | WAT V | 29 | 37.606 | 61.402 | 40.167 | 1.00 | 11.91 | 8 |
| 5403 | O24 | MAL A 691 | 30.444 | 73.291 | 70.263 | 1.00 | 19.15 | 8 | 5483 | OWO | WAT V | 30 | 16.372 | 70.863 | 38.933 | 1.00 | 11.99 | 8 |
| 5404 | C25 | MAL A 691 | 31.923 | 71.424 | 70.383 | 1.00 | 19.32 | 6 | 5484 | OWO | WAT V | 31 | 7.950 | 69.079 | 31.258 | 1.00 | 12.08 | 8 |
| 5405 | O25 | MAL A 691 | 32.521 | 70.374 | 69.608 | 1.00 | 18.98 | 8 | 5485 | OWO | WAT V | 32 | 19.528 | 73.999 | 43.164 | 1.00 | 12.10 | 8 |
| 5406 | C26 | MAL A 691 | 31.067 | 70.708 | 71.468 | 1.00 | 15.38 | 6 | 5486 | OWO | WAT V | 33 | 16.210 | 66.954 | 39.606 | 1.00 | 12.02 | 8 |
| 5407 | O26 | MAL A 691 | 31.944 | 70.075 | 72.412 | 1.00 | 18.74 | 8 | 5487 | OWO | WAT V | 34 | 32.679 | 63.267 | 29.330 | 1.00 | 12.26 | 8 |
| 5411 | S | SUL A 695 | 11.120 | 52.018 | 55.465 | 1.00 | 30.54 | 16 | 5488 | OWO | WAT V | 35 | 13.649 | 74.479 | 39.683 | 1.00 | 12.21 | 8 |
| 5412 | O1 | SUL A 695 | 11.470 | 52.936 | 56.533 | 1.00 | 30.07 | 8 | 5489 | OWO | WAT V | 36 | 16.357 | 79.631 | 22.013 | 1.00 | 12.26 | 8 |
| 5413 | O2 | SUL A 695 | 10.034 | 52.528 | 54.544 | 1.00 | 27.19 | 8 | 5490 | OWO | WAT V | 37 | 21.471 | 63.888 | 43.225 | 1.00 | 12.25 | 8 |
| 5414 | O3 | SUL A 695 | 12.310 | 51.631 | 54.662 | 1.00 | 34.25 | 8 | 5491 | OWO | WAT V | 38 | 42.464 | 66.587 | 23.881 | 1.00 | 12.49 | 8 |
| 5415 | O4 | SUL A 695 | 10.566 | 50.749 | 56.089 | 1.00 | 33.96 | 8 | 5492 | OWO | WAT V | 39 | 31.355 | 60.893 | 19.838 | 1.00 | 12.31 | 8 |
| 5451 | CA | WAT A 692 | 32.693 | 60.307 | 13.017 | 1.00 | 11.99 | 20 | 5493 | OWO | WAT V | 40 | 16.930 | 64.546 | 40.981 | 1.00 | 12.36 | 8 |
| 5452 | CA | WAT A 693 | 26.975 | 79.502 | 21.970 | 1.00 | 10.73 | 20 | 5494 | OWO | WAT V | 41 | 10.918 | 81.011 | 32.425 | 1.00 | 12.42 | 8 |
| 5453 | CA | WAT A 694 | 37.244 | 49.841 | 19.039 | 1.00 | 13.50 | 20 | 5495 | OWO | WAT V | 42 | 8.358 | 78.559 | 35.685 | 1.00 | 12.49 | 8 |
| 5454 | OWO | WAT V 1 | 24.447 | 79.971 | 21.858 | 1.00 | 9.43 | 8 | 5496 | OWO | WAT V | 43 | 22.052 | 71.621 | 41.190 | 1.00 | 12.24 | 8 |
| 5455 | OWO | WAT V 2 | 35.686 | 59.385 | 24.028 | 1.00 | 10.45 | 8 | 5497 | OWO | WAT V | 44 | 8.226 | 66.640 | 35.276 | 1.00 | 12.62 | 8 |
| 5456 | OWO | WAT V 3 | 33.934 | 60.773 | 18.648 | 1.00 | 10.63 | 8 | 5498 | OWO | WAT V | 45 | 6.031 | 77.562 | 36.868 | 1.00 | 12.35 | 8 |
| 5457 | OWO | WAT V 4 | 35.622 | 62.751 | 41.495 | 1.00 | 10.88 | 8 | 5499 | OWO | WAT V | 46 | 43.919 | 60.734 | 40.175 | 1.00 | 12.51 | 8 |
| 5458 | OWO | WAT V 5 | 25.780 | 77.914 | 20.486 | 1.00 | 10.75 | 8 | 5500 | OWO | WAT V | 48 | 11.578 | 73.478 | 41.191 | 1.00 | 12.62 | 8 |
| 5459 | OWO | WAT V 6 | 21.776 | 77.285 | 28.879 | 1.00 | 10.81 | 8 | 5501 | OWO | WAT V | 49 | 35.256 | 52.308 | 26.203 | 1.00 | 12.50 | 8 |
| 5460 | OWO | WAT V 7 | 29.415 | 69.145 | 19.400 | 1.00 | 10.86 | 8 | 5502 | OWO | WAT V | 50 | 22.628 | 81.739 | 22.782 | 1.00 | 12.52 | 8 |
| 5461 | OWO | WAT V 8 | 29.138 | 80.312 | 22.631 | 1.00 | 10.86 | 8 | 5503 | OWO | WAT V | 51 | 41.171 | 68.357 | 22.292 | 1.00 | 12.78 | 8 |
| 5462 | OWO | WAT V 9 | 27.613 | 72.037 | 24.448 | 1.00 | 10.77 | 8 | 5504 | OWO | WAT V | 52 | 34.554 | 71.110 | 10.783 | 1.00 | 12.58 | 8 |
| 5463 | OWO | WAT V 10 | 31.164 | 77.784 | 19.615 | 1.00 | 10.85 | 8 | 5505 | OWO | WAT V | 53 | 39.554 | 70.543 | 28.407 | 1.00 | 12.73 | 8 |
| 5464 | OWO | WAT V 11 | 32.790 | 66.917 | 36.378 | 1.00 | 10.94 | 8 | 5506 | OWO | WAT V | 54 | 14.970 | 66.671 | 43.779 | 1.00 | 12.94 | 8 |
| 5465 | OWO | WAT V 12 | 34.127 | 70.240 | 32.929 | 1.00 | 11.18 | 8 | 5507 | OWO | WAT V | 55 | 14.792 | 81.581 | 20.763 | 1.00 | 12.92 | 8 |
| 5466 | OWO | WAT V 13 | 33.080 | 60.581 | 23.767 | 1.00 | 11.11 | 8 | 5508 | OWO | WAT V | 56 | 30.205 | 75.643 | 31.109 | 1.00 | 12.90 | 8 |
| 5467 | OWO | WAT V 14 | 37.235 | 54.601 | 19.600 | 1.00 | 11.38 | 8 | 5509 | OWO | WAT V | 57 | 16.697 | 82.536 | 30.534 | 1.00 | 13.09 | 8 |
| 5468 | OWO | WAT V 15 | 26.119 | 65.542 | 21.574 | 1.00 | 11.07 | 8 | 5510 | OWO | WAT V | 58 | 38.776 | 53.289 | 57.732 | 1.00 | 13.10 | 8 |
| 5469 | OWO | WAT V 16 | 28.484 | 64.486 | 20.522 | 1.00 | 11.49 | 8 | 5511 | OWO | WAT V | 59 | 31.565 | 49.273 | 20.064 | 1.00 | 13.22 | 8 |
| 5470 | OWO | WAT V 17 | 28.194 | 73.536 | 36.853 | 1.00 | 11.53 | 8 | 5512 | OWO | WAT V | 60 | 20.200 | 85.147 | 36.037 | 1.00 | 13.29 | 8 |
| 5471 | OWO | WAT V 18 | 16.618 | 66.275 | 36.806 | 1.00 | 11.68 | 8 | 5513 | OWO | WAT V | 61 | 25.657 | 54.513 | 45.949 | 1.00 | 13.32 | 8 |

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|------|---------------|--------|--------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 5514 | OWO WAT V 62 | 37.048 | 52.273 | 18.284 | 1.00 | 13.46 | 8 | 5556 | OWO WAT V 104 | 14.144 | 58.009 | 41.510 | 1.00 | 15.84 | 8 |
| 5515 | OWO WAT V 63 | 30.032 | 67.305 | 53.938 | 1.00 | 13.27 | 8 | 5557 | OWO WAT V 105 | 44.010 | 71.623 | 35.990 | 1.00 | 15.89 | 8 |
| 5516 | OWO WAT V 64 | 32.331 | 68.357 | 33.829 | 1.00 | 13.58 | 8 | 5558 | OWO WAT V 106 | 21.168 | 82.474 | 32.738 | 1.00 | 16.12 | 8 |
| 5517 | OWO WAT V 65 | 23.329 | 85.511 | 30.252 | 1.00 | 13.33 | 8 | 5559 | OWO WAT V 107 | 28.667 | 48.688 | 46.155 | 1.00 | 16.35 | 8 |
| 5518 | OWO WAT V 66 | 20.246 | 61.387 | 18.981 | 1.00 | 13.61 | 8 | 5560 | OWO WAT V 108 | 25.610 | 86.818 | 38.209 | 1.00 | 16.18 | 8 |
| 5519 | OWO WAT V 67 | 28.775 | 74.856 | 40.336 | 1.00 | 13.65 | 8 | 5561 | OWO WAT V 109 | 29.070 | 89.992 | 31.492 | 1.00 | 16.47 | 8 |
| 5520 | OWO WAT V 68 | 32.567 | 68.924 | 43.607 | 1.00 | 13.35 | 8 | 5562 | OWO WAT V 110 | 1.291 | 75.000 | 41.091 | 1.00 | 16.32 | 8 |
| 5521 | OWO WAT V 69 | 10.838 | 68.713 | 42.880 | 1.00 | 13.33 | 8 | 5563 | OWO WAT V 111 | 34.624 | 56.600 | 71.328 | 1.00 | 16.34 | 8 |
| 5522 | OWO WAT V 70 | 12.859 | 61.518 | 43.606 | 1.00 | 13.90 | 8 | 5564 | OWO WAT V 112 | 28.281 | 69.481 | 68.152 | 1.00 | 16.52 | 8 |
| 5523 | OWO WAT V 71 | 45.207 | 60.214 | 32.334 | 1.00 | 13.77 | 8 | 5565 | OWO WAT V 113 | 26.135 | 87.038 | 35.304 | 1.00 | 16.58 | 8 |
| 5524 | OWO WAT V 72 | 27.427 | 66.987 | 53.108 | 1.00 | 13.75 | 8 | 5566 | OWO WAT V 114 | 35.168 | 78.123 | 51.153 | 1.00 | 16.64 | 8 |
| 5525 | OWO WAT V 73 | 19.074 | 63.276 | 42.264 | 1.00 | 13.66 | 8 | 5567 | OWO WAT V 115 | 19.827 | 81.281 | 46.203 | 1.00 | 16.48 | 8 |
| 5526 | OWO WAT V 74 | 36.934 | 75.592 | 8.270 | 1.00 | 13.53 | 8 | 5568 | OWO WAT V 116 | 30.082 | 84.087 | 8.323 | 1.00 | 16.75 | 8 |
| 5527 | OWO WAT V 75 | 27.574 | 81.410 | 6.013 | 1.00 | 14.19 | 8 | 5569 | OWO WAT V 117 | 45.164 | 71.238 | 15.992 | 1.00 | 16.58 | 8 |
| 5528 | OWO WAT V 76 | 30.621 | 83.670 | 31.215 | 1.00 | 14.28 | 8 | 5570 | OWO WAT V 118 | -2.555 | 86.829 | 29.585 | 1.00 | 16.73 | 8 |
| 5529 | OWO WAT V 77 | 42.514 | 70.356 | 20.822 | 1.00 | 14.45 | 8 | 5571 | OWO WAT V 119 | 1.879 | 75.860 | 26.297 | 1.00 | 16.96 | 8 |
| 5530 | OWO WAT V 78 | 12.529 | 75.168 | 22.815 | 1.00 | 14.52 | 8 | 5572 | OWO WAT V 120 | 20.960 | 94.415 | 22.713 | 1.00 | 16.87 | 8 |
| 5531 | OWO WAT V 79 | 39.891 | 56.461 | 11.992 | 1.00 | 14.18 | 8 | 5573 | OWO WAT V 121 | 12.300 | 72.626 | 21.951 | 1.00 | 16.94 | 8 |
| 5532 | OWO WAT V 80 | 30.677 | 68.114 | 68.620 | 1.00 | 14.47 | 8 | 5574 | OWO WAT V 122 | 21.720 | 86.954 | 37.648 | 1.00 | 17.08 | 8 |
| 5533 | OWO WAT V 81 | 33.218 | 64.224 | 36.711 | 1.00 | 14.46 | 8 | 5575 | OWO WAT V 123 | 17.342 | 46.052 | 29.967 | 1.00 | 16.89 | 8 |
| 5534 | OWO WAT V 82 | 12.035 | 74.811 | 37.533 | 1.00 | 14.63 | 8 | 5576 | OWO WAT V 124 | 15.847 | 84.337 | 34.562 | 1.00 | 16.74 | 8 |
| 5535 | OWO WAT V 83 | 15.981 | 73.538 | 38.669 | 1.00 | 14.16 | 8 | 5577 | OWO WAT V 125 | -3.241 | 60.294 | 45.682 | 1.00 | 16.67 | 8 |
| 5536 | OWO WAT V 84 | 10.686 | 81.113 | 35.947 | 1.00 | 14.90 | 8 | 5578 | OWO WAT V 126 | 11.587 | 104.148 | 24.323 | 1.00 | 17.24 | 8 |
| 5537 | OWO WAT V 85 | 25.562 | 71.871 | 51.287 | 1.00 | 14.81 | 8 | 5579 | OWO WAT V 127 | 28.501 | 56.852 | 51.441 | 1.00 | 17.40 | 8 |
| 5538 | OWO WAT V 86 | 29.447 | 83.564 | 16.644 | 1.00 | 14.86 | 8 | 5580 | OWO WAT V 128 | 14.206 | 82.937 | 18.392 | 1.00 | 17.21 | 8 |
| 5539 | OWO WAT V 87 | 13.480 | 81.300 | 31.112 | 1.00 | 14.85 | 8 | 5581 | OWO WAT V 129 | 41.516 | 56.407 | 63.525 | 1.00 | 17.22 | 8 |
| 5540 | OWO WAT V 88 | 5.774 | 80.076 | 41.775 | 1.00 | 14.92 | 8 | 5582 | OWO WAT V 130 | 36.936 | 73.986 | 40.016 | 1.00 | 17.65 | 8 |
| 5541 | OWO WAT V 89 | 47.914 | 63.828 | 68.644 | 1.00 | 14.87 | 8 | 5583 | OWO WAT V 131 | 20.790 | 40.115 | 27.752 | 1.00 | 17.53 | 8 |
| 5542 | OWO WAT V 90 | 34.743 | 77.662 | 45.101 | 1.00 | 15.02 | 8 | 5584 | OWO WAT V 132 | 45.240 | 52.146 | 20.212 | 1.00 | 17.55 | 8 |
| 5543 | OWO WAT V 91 | 24.427 | 76.387 | 7.359 | 1.00 | 15.03 | 8 | 5585 | OWO WAT V 133 | 41.799 | 49.726 | 28.892 | 1.00 | 17.29 | 8 |
| 5544 | OWO WAT V 92 | -2.703 | 63.471 | 38.845 | 1.00 | 15.46 | 8 | 5586 | OWO WAT V 134 | 23.108 | 66.755 | 60.083 | 1.00 | 17.41 | 8 |
| 5545 | OWO WAT V 93 | 14.681 | 69.092 | 37.625 | 1.00 | 15.14 | 8 | 5587 | OWO WAT V 135 | 26.863 | 48.805 | 41.435 | 1.00 | 17.67 | 8 |
| 5546 | OWO WAT V 94 | 28.123 | 74.474 | 42.954 | 1.00 | 15.12 | 8 | 5588 | OWO WAT V 136 | 27.488 | 90.699 | 28.339 | 1.00 | 17.76 | 8 |
| 5547 | OWO WAT V 95 | 23.589 | 80.407 | 29.737 | 1.00 | 15.19 | 8 | 5589 | OWO WAT V 137 | 0.191 | 69.111 | 49.096 | 1.00 | 17.78 | 8 |
| 5548 | OWO WAT V 96 | 28.941 | 64.658 | 47.281 | 1.00 | 15.32 | 8 | 5590 | OWO WAT V 138 | 34.447 | 43.232 | 33.946 | 1.00 | 17.85 | 8 |
| 5549 | OWO WAT V 97 | 33.848 | 82.923 | 7.441 | 1.00 | 15.09 | 8 | 5591 | OWO WAT V 139 | 22.589 | 64.044 | 49.415 | 1.00 | 18.18 | 8 |
| 5550 | OWO WAT V 98 | 50.687 | 59.709 | 65.034 | 1.00 | 15.32 | 8 | 5592 | OWO WAT V 140 | 17.697 | 81.339 | 35.462 | 1.00 | 17.98 | 8 |
| 5551 | OWO WAT V 99 | 29.977 | 80.264 | 14.804 | 1.00 | 15.36 | 8 | 5593 | OWO WAT V 141 | 2.444 | 96.838 | 37.934 | 1.00 | 18.09 | 8 |
| 5552 | OWO WAT V 100 | 25.916 | 52.607 | 44.011 | 1.00 | 15.58 | 8 | 5594 | OWO WAT V 142 | 35.347 | 81.251 | 39.545 | 1.00 | 17.94 | 8 |
| 5553 | OWO WAT V 101 | 6.765 | 62.176 | 32.083 | 1.00 | 15.56 | 8 | 5595 | OWO WAT V 143 | 14.511 | 56.297 | 49.652 | 1.00 | 18.35 | 8 |
| 5554 | OWO WAT V 102 | 13.107 | 89.810 | 20.076 | 1.00 | 15.94 | 8 | 5596 | OWO WAT V 144 | 10.014 | 71.654 | 20.618 | 1.00 | 18.11 | 8 |
| 5555 | OWO WAT V 103 | 11.601 | 78.292 | 36.745 | 1.00 | 15.75 | 8 | 5597 | OWO WAT V 145 | 47.629 | 63.815 | 18.991 | 1.00 | 18.25 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|--------|--------|------|-------|---|
| 5598 | OWO WAT V 146 | 15.832 | 79.962 | 31.635 | 1.00 | 18.52 | 8 | 5640 | OWO WAT V 195 | 43.898 | 69.204 | 9.296 | 1.00 | 20.35 | 8 |
| 5599 | OWO WAT V 147 | 35.482 | 76.428 | 39.594 | 1.00 | 18.64 | 8 | 5641 | OWO WAT V 196 | 17.503 | 91.553 | 19.944 | 1.00 | 20.36 | 8 |
| 5600 | OWO WAT V 149 | 16.532 | 67.334 | 48.159 | 1.00 | 18.61 | 8 | 5642 | OWO WAT V 197 | 22.079 | 71.014 | 56.203 | 1.00 | 20.50 | 8 |
| 5601 | OWO WAT V 150 | 32.280 | 83.173 | 33.550 | 1.00 | 18.44 | 8 | 5643 | OWO WAT V 198 | 24.611 | 90.278 | 32.659 | 1.00 | 20.71 | 8 |
| 5602 | OWO WAT V 151 | 35.037 | 62.885 | 71.628 | 1.00 | 18.62 | 8 | 5644 | OWO WAT V 199 | 15.822 | 79.667 | 34.285 | 1.00 | 20.71 | 8 |
| 5603 | OWO WAT V 152 | 14.756 | 56.448 | 28.743 | 1.00 | 18.87 | 8 | 5645 | OWO WAT V 200 | 41.507 | 64.519 | 35.769 | 1.00 | 20.47 | 8 |
| 5604 | OWO WAT V 153 | 51.007 | 64.138 | 32.515 | 1.00 | 18.45 | 8 | 5646 | OWO WAT V 201 | 50.582 | 63.510 | 21.444 | 1.00 | 20.44 | 8 |
| 5605 | OWO WAT V 154 | 44.683 | 55.406 | 52.749 | 1.00 | 18.86 | 8 | 5647 | OWO WAT V 202 | -4.254 | 88.781 | 28.481 | 1.00 | 20.69 | 8 |
| 5606 | OWO WAT V 155 | 30.803 | 47.286 | 18.413 | 1.00 | 19.00 | 8 | 5648 | OWO WAT V 203 | 41.289 | 48.120 | 25.349 | 1.00 | 20.50 | 8 |
| 5607 | OWO WAT V 156 | 21.419 | 87.008 | 31.586 | 1.00 | 18.86 | 8 | 5649 | OWO WAT V 204 | 33.838 | 47.522 | 55.491 | 1.00 | 20.42 | 8 |
| 5608 | OWO WAT V 157 | 27.471 | 54.562 | 13.822 | 1.00 | 18.93 | 8 | 5650 | OWO WAT V 205 | 28.696 | 42.611 | 30.481 | 1.00 | 21.10 | 8 |
| 5609 | OWO WAT V 158 | 19.938 | 85.031 | 32.888 | 1.00 | 18.77 | 8 | 5651 | OWO WAT V 206 | 29.680 | 89.479 | 34.207 | 1.00 | 20.71 | 8 |
| 5610 | OWO WAT V 160 | 23.159 | 58.927 | 72.012 | 1.00 | 19.01 | 8 | 5652 | OWO WAT V 207 | 13.375 | 82.989 | 38.528 | 1.00 | 20.79 | 8 |
| 5611 | OWO WAT V 161 | 20.470 | 84.773 | 18.243 | 1.00 | 19.09 | 8 | 5653 | OWO WAT V 208 | -0.381 | 94.652 | 35.925 | 1.00 | 20.71 | 8 |
| 5612 | OWO WAT V 162 | 15.077 | 66.831 | 13.792 | 1.00 | 18.88 | 8 | 5654 | OWO WAT V 209 | 32.894 | 53.249 | 7.401 | 1.00 | 20.79 | 8 |
| 5613 | OWO WAT V 164 | 34.016 | 76.548 | 58.886 | 1.00 | 19.18 | 8 | 5655 | OWO WAT V 210 | 47.202 | 71.009 | 63.961 | 1.00 | 20.83 | 8 |
| 5614 | OWO WAT V 165 | 1.791 | 96.077 | 35.490 | 1.00 | 19.39 | 8 | 5656 | OWO WAT V 211 | 16.432 | 73.589 | 49.935 | 1.00 | 20.64 | 8 |
| 5615 | OWO WAT V 168 | 16.921 | 65.681 | 50.173 | 1.00 | 19.74 | 8 | 5657 | OWO WAT V 212 | 36.761 | 42.123 | 23.718 | 1.00 | 20.49 | 8 |
| 5616 | OWO WAT V 169 | 36.015 | 49.508 | 63.823 | 1.00 | 19.75 | 8 | 5658 | OWO WAT V 213 | 1.326 | 98.176 | 25.977 | 1.00 | 21.14 | 8 |
| 5617 | OWO WAT V 170 | 19.146 | 93.639 | 20.716 | 1.00 | 19.72 | 8 | 5659 | OWO WAT V 215 | 32.369 | 84.143 | 13.694 | 1.00 | 21.27 | 8 |
| 5618 | OWO WAT V 171 | 41.081 | 74.262 | 43.114 | 1.00 | 19.99 | 8 | 5660 | OWO WAT V 216 | 1.000 | 72.006 | 27.168 | 1.00 | 21.23 | 8 |
| 5619 | OWO WAT V 172 | 27.356 | 86.834 | 41.150 | 1.00 | 19.86 | 8 | 5661 | OWO WAT V 217 | 21.907 | 50.669 | 62.000 | 1.00 | 21.19 | 8 |
| 5620 | OWO WAT V 173 | 32.541 | 61.241 | 6.239 | 1.00 | 19.49 | 8 | 5662 | OWO WAT V 218 | 30.956 | 41.738 | 21.314 | 1.00 | 21.03 | 8 |
| 5621 | OWO WAT V 174 | 51.971 | 65.011 | 17.317 | 1.00 | 20.07 | 8 | 5663 | OWO WAT V 219 | 36.121 | 71.463 | 4.684 | 1.00 | 21.46 | 8 |
| 5622 | OWO WAT V 175 | 36.754 | 79.161 | 49.332 | 1.00 | 19.96 | 8 | 5664 | OWO WAT V 220 | 13.404 | 81.016 | 34.970 | 1.00 | 21.65 | 8 |
| 5623 | OWO WAT V 176 | 21.529 | 68.516 | 52.600 | 1.00 | 19.88 | 8 | 5665 | OWO WAT V 221 | 22.957 | 65.844 | 62.604 | 1.00 | 21.35 | 8 |
| 5624 | OWO WAT V 177 | 52.175 | 64.476 | 48.627 | 1.00 | 19.48 | 8 | 5666 | OWO WAT V 222 | 4.260 | 99.337 | 39.649 | 1.00 | 21.63 | 8 |
| 5625 | OWO WAT V 178 | 47.687 | 55.894 | 28.556 | 1.00 | 19.85 | 8 | 5667 | OWO WAT V 223 | 17.535 | 84.263 | 32.555 | 1.00 | 20.98 | 8 |
| 5626 | OWO WAT V 180 | 28.309 | 57.733 | 12.302 | 1.00 | 19.86 | 8 | 5668 | OWO WAT V 224 | 16.496 | 59.065 | 45.746 | 1.00 | 21.66 | 8 |
| 5627 | OWO WAT V 181 | 19.852 | 88.585 | 39.017 | 1.00 | 20.03 | 8 | 5669 | OWO WAT V 225 | 16.576 | 52.574 | 34.164 | 1.00 | 21.65 | 8 |
| 5628 | OWO WAT V 182 | 48.116 | 65.053 | 11.253 | 1.00 | 19.75 | 8 | 5670 | OWO WAT V 226 | 30.825 | 51.406 | 13.432 | 1.00 | 21.28 | 8 |
| 5629 | OWO WAT V 183 | 45.728 | 49.401 | 46.755 | 1.00 | 20.07 | 8 | 5671 | OWO WAT V 227 | 39.177 | 82.848 | 23.121 | 1.00 | 21.63 | 8 |
| 5630 | OWO WAT V 184 | 23.090 | 51.403 | 56.173 | 1.00 | 19.76 | 8 | 5672 | OWO WAT V 229 | 19.108 | 58.790 | 36.143 | 1.00 | 21.40 | 8 |
| 5631 | OWO WAT V 185 | 23.972 | 69.604 | 53.226 | 1.00 | 20.10 | 8 | 5673 | OWO WAT V 230 | 19.087 | 75.378 | 50.063 | 1.00 | 21.22 | 8 |
| 5632 | OWO WAT V 186 | 49.679 | 65.500 | 55.245 | 1.00 | 19.98 | 8 | 5674 | OWO WAT V 231 | 47.413 | 69.881 | 16.583 | 1.00 | 21.29 | 8 |
| 5633 | OWO WAT V 187 | 50.720 | 57.388 | 48.688 | 1.00 | 20.39 | 8 | 5675 | OWO WAT V 232 | 26.686 | 91.040 | 31.058 | 1.00 | 21.61 | 8 |
| 5634 | OWO WAT V 188 | 34.857 | 63.152 | 38.228 | 1.00 | 20.23 | 8 | 5676 | OWO WAT V 233 | 29.036 | 52.089 | 61.852 | 1.00 | 21.25 | 8 |
| 5635 | OWO WAT V 189 | 37.511 | 43.029 | 19.233 | 1.00 | 20.32 | 8 | 5677 | OWO WAT V 234 | 36.187 | 79.293 | 46.671 | 1.00 | 21.45 | 8 |
| 5636 | OWO WAT V 190 | 50.567 | 67.974 | 10.449 | 1.00 | 20.64 | 8 | 5678 | OWO WAT V 235 | 37.289 | 74.835 | 65.582 | 1.00 | 21.65 | 8 |
| 5637 | OWO WAT V 191 | 29.875 | 92.014 | 24.922 | 1.00 | 20.34 | 8 | 5679 | OWO WAT V 236 | -0.428 | 68.770 | 30.109 | 1.00 | 21.94 | 8 |
| 5638 | OWO WAT V 192 | 4.055 | 100.811 | 36.567 | 1.00 | 20.35 | 8 | 5680 | OWO WAT V 237 | 50.762 | 57.829 | 44.061 | 1.00 | 22.15 | 8 |
| 5639 | OWO WAT V 194 | 23.592 | 87.859 | 32.780 | 1.00 | 20.02 | 8 | 5681 | OWO WAT V 238 | 45.167 | 70.565 | 24.893 | 1.00 | 22.00 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 5682 | OWO WAT V 239 | 28.609 | 48.609 | 51.930 | 1.00 | 22.03 | 8 | 5724 | OWO WAT V 282 | 13.480 | 62.142 | 18.325 | 1.00 | 23.48 | 8 |
| 5683 | OWO WAT V 241 | 2.366 | 94.552 | 38.603 | 1.00 | 21.97 | 8 | 5725 | OWO WAT V 283 | 19.332 | 56.925 | 43.429 | 1.00 | 23.84 | 8 |
| 5684 | OWO WAT V 242 | 9.365 | 68.970 | 20.742 | 1.00 | 22.04 | 8 | 5726 | OWO WAT V 284 | 7.117 | 53.127 | 42.902 | 1.00 | 23.57 | 8 |
| 5685 | OWO WAT V 243 | 38.583 | 85.642 | 29.447 | 1.00 | 21.90 | 8 | 5727 | OWO WAT V 285 | 27.829 | 78.220 | 46.852 | 1.00 | 24.20 | 8 |
| 5686 | OWO WAT V 244 | 24.639 | 49.542 | 55.081 | 1.00 | 22.42 | 8 | 5728 | OWO WAT V 286 | 49.295 | 57.105 | 51.124 | 1.00 | 23.77 | 8 |
| 5687 | OWO WAT V 245 | 18.177 | 95.474 | 18.838 | 1.00 | 22.69 | 8 | 5729 | OWO WAT V 287 | 13.680 | 105.356 | 27.022 | 1.00 | 24.03 | 8 |
| 5688 | OWO WAT V 246 | 37.307 | 43.276 | 33.862 | 1.00 | 22.90 | 8 | 5730 | OWO WAT V 288 | 17.824 | 106.639 | 32.939 | 1.00 | 24.44 | 8 |
| 5689 | OWO WAT V 247 | 23.478 | 86.290 | 16.425 | 1.00 | 21.85 | 8 | 5731 | OWO WAT V 289 | 15.542 | 66.715 | 53.507 | 1.00 | 24.42 | 8 |
| 5690 | OWO WAT V 248 | 43.569 | 60.466 | 72.156 | 1.00 | 23.10 | 8 | 5732 | OWO WAT V 290 | 27.050 | 47.324 | 23.573 | 1.00 | 24.19 | 8 |
| 5691 | OWO WAT V 249 | 23.281 | 40.658 | 26.691 | 1.00 | 22.77 | 8 | 5733 | OWO WAT V 291 | 39.482 | 73.577 | 31.816 | 1.00 | 24.19 | 8 |
| 5692 | OWO WAT V 250 | 8.761 | 65.837 | 24.376 | 1.00 | 23.00 | 8 | 5734 | OWO WAT V 292 | 10.356 | 77.638 | 16.052 | 1.00 | 23.96 | 8 |
| 5693 | OWO WAT V 251 | 27.215 | 72.803 | 60.509 | 1.00 | 22.60 | 8 | 5735 | OWO WAT V 293 | 24.405 | 50.730 | 63.252 | 1.00 | 24.31 | 8 |
| 5694 | OWO WAT V 252 | 16.174 | 91.014 | 44.772 | 1.00 | 22.53 | 8 | 5736 | OWO WAT V 294 | 15.639 | 54.776 | 31.091 | 1.00 | 24.31 | 8 |
| 5695 | OWO WAT V 253 | 3.297 | 98.395 | 35.969 | 1.00 | 23.15 | 8 | 5737 | OWO WAT V 295 | -5.196 | 74.449 | 41.013 | 1.00 | 24.22 | 8 |
| 5696 | OWO WAT V 254 | 10.918 | 68.974 | 53.447 | 1.00 | 23.22 | 8 | 5738 | OWO WAT V 296 | 40.985 | 72.335 | 29.872 | 1.00 | 24.55 | 8 |
| 5697 | OWO WAT V 255 | -5.802 | 66.167 | 37.375 | 1.00 | 23.15 | 8 | 5739 | OWO WAT V 297 | 48.449 | 77.051 | 18.858 | 1.00 | 24.18 | 8 |
| 5698 | OWO WAT V 256 | 8.490 | 91.603 | 44.099 | 1.00 | 22.65 | 8 | 5740 | OWO WAT V 298 | 25.992 | 92.521 | 26.784 | 1.00 | 24.84 | 8 |
| 5699 | OWO WAT V 257 | 9.234 | 73.507 | 16.552 | 1.00 | 22.92 | 8 | 5741 | OWO WAT V 299 | 45.814 | 49.306 | 39.112 | 1.00 | 24.65 | 8 |
| 5700 | OWO WAT V 258 | 15.730 | 56.257 | 16.556 | 1.00 | 23.08 | 8 | 5742 | OWO WAT V 300 | 44.725 | 55.968 | 11.440 | 1.00 | 24.73 | 8 |
| 5701 | OWO WAT V 259 | 19.989 | 82.268 | 13.713 | 1.00 | 22.90 | 8 | 5743 | OWO WAT V 301 | 20.058 | 84.809 | 46.357 | 1.00 | 24.94 | 8 |
| 5702 | OWO WAT V 260 | 27.613 | 49.792 | 60.562 | 1.00 | 23.09 | 8 | 5744 | OWO WAT V 302 | 18.079 | 50.984 | 17.334 | 1.00 | 24.58 | 8 |
| 5703 | OWO WAT V 261 | 26.408 | 61.061 | 10.006 | 1.00 | 23.11 | 8 | 5745 | OWO WAT V 303 | 17.020 | 65.666 | 56.879 | 1.00 | 24.81 | 8 |
| 5704 | OWO WAT V 262 | 14.277 | 70.834 | 12.781 | 1.00 | 23.32 | 8 | 5746 | OWO WAT V 304 | 44.682 | 72.661 | 22.319 | 1.00 | 24.66 | 8 |
| 5705 | OWO WAT V 263 | -3.969 | 72.948 | 34.601 | 1.00 | 22.98 | 8 | 5747 | OWO WAT V 305 | 0.091 | 75.457 | 45.401 | 1.00 | 24.37 | 8 |
| 5706 | OWO WAT V 264 | -1.028 | 93.829 | 38.475 | 1.00 | 23.17 | 8 | 5748 | OWO WAT V 306 | 50.222 | 58.393 | 53.380 | 1.00 | 24.90 | 8 |
| 5707 | OWO WAT V 265 | 19.230 | 101.476 | 27.805 | 1.00 | 22.95 | 8 | 5749 | OWO WAT V 307 | 44.639 | 52.674 | 53.486 | 1.00 | 25.29 | 8 |
| 5708 | OWO WAT V 266 | 17.914 | 54.281 | 55.523 | 1.00 | 23.31 | 8 | 5750 | OWO WAT V 308 | 49.725 | 64.827 | 52.493 | 1.00 | 24.60 | 8 |
| 5709 | OWO WAT V 267 | -1.163 | 64.024 | 50.895 | 1.00 | 23.41 | 8 | 5751 | OWO WAT V 309 | 39.542 | 61.118 | 7.698 | 1.00 | 24.82 | 8 |
| 5710 | OWO WAT V 268 | 16.209 | 48.607 | 29.481 | 1.00 | 23.45 | 8 | 5752 | OWO WAT V 310 | 41.190 | 79.148 | 23.073 | 1.00 | 25.15 | 8 |
| 5711 | OWO WAT V 269 | 35.070 | 63.595 | 75.008 | 1.00 | 23.90 | 8 | 5753 | OWO WAT V 311 | 1.598 | 80.899 | 39.623 | 1.00 | 24.95 | 8 |
| 5712 | OWO WAT V 270 | 38.343 | 43.626 | 21.918 | 1.00 | 23.33 | 8 | 5754 | OWO WAT V 312 | 25.053 | 45.139 | 19.817 | 1.00 | 24.92 | 8 |
| 5713 | OWO WAT V 271 | 32.197 | 85.153 | 37.181 | 1.00 | 23.49 | 8 | 5755 | OWO WAT V 313 | 16.135 | 84.191 | 47.663 | 1.00 | 25.20 | 8 |
| 5714 | OWO WAT V 272 | 28.789 | 71.419 | 66.331 | 1.00 | 22.79 | 8 | 5756 | OWO WAT V 314 | 11.381 | 71.857 | 49.110 | 1.00 | 25.29 | 8 |
| 5715 | OWO WAT V 273 | 41.806 | 79.697 | 18.591 | 1.00 | 23.39 | 8 | 5757 | OWO WAT V 315 | -4.512 | 57.278 | 42.326 | 1.00 | 25.43 | 8 |
| 5716 | OWO WAT V 274 | 38.127 | 43.105 | 36.443 | 1.00 | 23.39 | 8 | 5758 | OWO WAT V 316 | 3.805 | 93.061 | 22.790 | 1.00 | 25.09 | 8 |
| 5717 | OWO WAT V 275 | 16.104 | 65.021 | 59.364 | 1.00 | 23.44 | 8 | 5759 | OWO WAT V 317 | 34.832 | 82.782 | 37.221 | 1.00 | 25.16 | 8 |
| 5718 | OWO WAT V 276 | -6.314 | 69.710 | 39.367 | 1.00 | 24.17 | 8 | 5760 | OWO WAT V 318 | 3.711 | 95.706 | 23.179 | 1.00 | 25.31 | 8 |
| 5719 | OWO WAT V 277 | 25.476 | 86.458 | 13.742 | 1.00 | 23.04 | 8 | 5761 | OWO WAT V 319 | 20.209 | 70.499 | 54.469 | 1.00 | 25.69 | 8 |
| 5720 | OWO WAT V 278 | 0.680 | 86.883 | 37.755 | 1.00 | 23.27 | 8 | 5762 | OWO WAT V 320 | 11.697 | 68.339 | 56.789 | 1.00 | 25.01 | 8 |
| 5721 | OWO WAT V 279 | 33.015 | 81.157 | 29.976 | 1.00 | 23.30 | 8 | 5763 | OWO WAT V 321 | 7.254 | 91.019 | 18.448 | 1.00 | 25.40 | 8 |
| 5722 | OWO WAT V 280 | 1.763 | 88.744 | 19.524 | 1.00 | 23.68 | 8 | 5764 | OWO WAT V 322 | 42.661 | 49.979 | 21.111 | 1.00 | 25.81 | 8 |
| 5723 | OWO WAT V 281 | 13.574 | 55.293 | 46.773 | 1.00 | 23.63 | 8 | 5765 | OWO WAT V 323 | 17.078 | 70.892 | 50.293 | 1.00 | 25.51 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 5766 | OWO WAT V 324 | 49.200 | 60.915 | 31.600 | 1.00 | 25.53 | 8 | 5808 | OWO WAT V 366 | 30.943 | 49.068 | 15.778 | 1.00 | 26.98 | 8 |
| 5767 | OWO WAT V 325 | 31.661 | 71.214 | 4.552 | 1.00 | 25.64 | 8 | 5809 | OWO WAT V 367 | 43.193 | 44.166 | 34.878 | 1.00 | 26.97 | 8 |
| 5768 | OWO WAT V 326 | -2.062 | 96.310 | 27.990 | 1.00 | 25.87 | 8 | 5810 | OWO WAT V 368 | 6.994 | 74.430 | 21.876 | 1.00 | 27.26 | 8 |
| 5769 | OWO WAT V 327 | 39.125 | 80.230 | 56.164 | 1.00 | 26.25 | 8 | 5811 | OWO WAT V 369 | 34.427 | 88.111 | 38.939 | 1.00 | 27.30 | 8 |
| 5770 | OWO WAT V 328 | 48.433 | 70.294 | 57.525 | 1.00 | 25.87 | 8 | 5812 | OWO WAT V 370 | 1.636 | 93.582 | 40.791 | 1.00 | 27.54 | 8 |
| 5771 | OWO WAT V 329 | -2.772 | 64.990 | 34.941 | 1.00 | 25.71 | 8 | 5813 | OWO WAT V 371 | 5.971 | 98.241 | 21.504 | 1.00 | 27.42 | 8 |
| 5772 | OWO WAT V 330 | 35.352 | 40.001 | 22.353 | 1.00 | 25.96 | 8 | 5814 | OWO WAT V 372 | 29.223 | 75.038 | 60.445 | 1.00 | 26.93 | 8 |
| 5773 | OWO WAT V 331 | 34.557 | 81.627 | 46.792 | 1.00 | 26.23 | 8 | 5815 | OWO WAT V 373 | 31.316 | 53.650 | 9.481 | 1.00 | 27.85 | 8 |
| 5774 | OWO WAT V 332 | 23.250 | 92.581 | 31.676 | 1.00 | 26.20 | 8 | 5816 | OWO WAT V 374 | 43.939 | 56.548 | 55.050 | 1.00 | 27.63 | 8 |
| 5775 | OWO WAT V 333 | 23.167 | 53.251 | 13.715 | 1.00 | 25.74 | 8 | 5817 | OWO WAT V 375 | 46.559 | 74.427 | 54.610 | 1.00 | 27.46 | 8 |
| 5776 | OWO WAT V 334 | 20.707 | 52.356 | 39.202 | 1.00 | 25.65 | 8 | 5818 | OWO WAT V 376 | 26.961 | 70.400 | 70.205 | 1.00 | 28.10 | 8 |
| 5777 | OWO WAT V 335 | 4.870 | 93.727 | 41.264 | 1.00 | 26.54 | 8 | 5819 | OWO WAT V 377 | 48.989 | 57.080 | 35.445 | 1.00 | 28.37 | 8 |
| 5778 | OWO WAT V 336 | 0.053 | 71.401 | 29.885 | 1.00 | 25.67 | 8 | 5820 | OWO WAT V 378 | 14.950 | 47.050 | 27.899 | 1.00 | 27.90 | 8 |
| 5779 | OWO WAT V 337 | 20.015 | 56.517 | 72.324 | 1.00 | 25.86 | 8 | 5821 | OWO WAT V 379 | 46.760 | 46.713 | 39.616 | 1.00 | 27.67 | 8 |
| 5780 | OWO WAT V 338 | 13.826 | 74.132 | 49.507 | 1.00 | 26.36 | 8 | 5822 | OWO WAT V 380 | -1.380 | 79.896 | 38.771 | 1.00 | 28.02 | 8 |
| 5781 | OWO WAT V 339 | 44.958 | 71.632 | 28.685 | 1.00 | 26.80 | 8 | 5823 | OWO WAT V 381 | 12.690 | 81.625 | 15.826 | 1.00 | 28.03 | 8 |
| 5782 | OWO WAT V 340 | -0.093 | 73.784 | 33.119 | 1.00 | 26.07 | 8 | 5824 | OWO WAT V 382 | 10.617 | 104.039 | 32.646 | 1.00 | 28.19 | 8 |
| 5784 | OWO WAT V 341 | 49.630 | 56.579 | 40.106 | 1.00 | 26.64 | 8 | 5825 | OWO WAT V 383 | 13.859 | 80.594 | 13.625 | 1.00 | 27.99 | 8 |
| 5785 | OWO WAT V 342 | 15.628 | 79.186 | 45.524 | 1.00 | 26.42 | 8 | 5826 | OWO WAT V 384 | 7.322 | 72.231 | 20.822 | 1.00 | 28.35 | 8 |
| 5786 | OWO WAT V 343 | 31.176 | 91.867 | 30.769 | 1.00 | 26.10 | 8 | 5827 | OWO WAT V 385 | 29.284 | 46.632 | 44.658 | 1.00 | 28.26 | 8 |
| 5787 | OWO WAT V 344 | 15.626 | 67.643 | 55.543 | 1.00 | 26.46 | 8 | 5828 | OWO WAT V 386 | 18.064 | 50.559 | 24.862 | 1.00 | 28.35 | 8 |
| 5788 | OWO WAT V 345 | 21.398 | 95.678 | 38.839 | 1.00 | 26.79 | 8 | 5829 | OWO WAT V 387 | 35.054 | 45.412 | 46.835 | 1.00 | 28.58 | 8 |
| 5789 | OWO WAT V 346 | 41.099 | 41.982 | 39.915 | 1.00 | 26.66 | 8 | 5830 | OWO WAT V 388 | 22.478 | 83.558 | 13.277 | 1.00 | 28.32 | 8 |
| 5790 | OWO WAT V 347 | 22.442 | 79.888 | 2.661 | 1.00 | 26.18 | 8 | 5831 | OWO WAT V 389 | 10.928 | 67.510 | 14.236 | 1.00 | 28.65 | 8 |
| 5791 | OWO WAT V 348 | 44.448 | 72.532 | 39.099 | 1.00 | 27.08 | 8 | 5832 | OWO WAT V 390 | 33.397 | 82.246 | 49.220 | 1.00 | 27.37 | 8 |
| 5792 | OWO WAT V 349 | 40.265 | 82.719 | 10.175 | 1.00 | 26.27 | 8 | 5833 | OWO WAT V 391 | 23.434 | 88.556 | 18.508 | 1.00 | 28.95 | 8 |
| 5793 | OWO WAT V 350 | 40.934 | 43.657 | 30.662 | 1.00 | 27.04 | 8 | 5834 | OWO WAT V 392 | 29.832 | 42.212 | 39.251 | 1.00 | 28.21 | 8 |
| 5794 | OWO WAT V 351 | -1.666 | 97.213 | 32.163 | 1.00 | 27.31 | 8 | 5835 | OWO WAT V 393 | 15.076 | 70.102 | 51.758 | 1.00 | 27.91 | 8 |
| 5795 | OWO WAT V 352 | -8.111 | 67.221 | 45.293 | 1.00 | 27.12 | 8 | 5836 | OWO WAT V 394 | 35.566 | 48.453 | 66.263 | 1.00 | 28.16 | 8 |
| 5796 | OWO WAT V 353 | 16.355 | 56.614 | 42.471 | 1.00 | 27.10 | 8 | 5837 | OWO WAT V 395 | 34.691 | 46.594 | 49.301 | 1.00 | 28.85 | 8 |
| 5797 | OWO WAT V 354 | 11.346 | 65.531 | 19.934 | 1.00 | 27.40 | 8 | 5838 | OWO WAT V 396 | 39.702 | 74.440 | 36.238 | 1.00 | 28.77 | 8 |
| 5798 | OWO WAT V 355 | 11.189 | 105.275 | 21.949 | 1.00 | 27.29 | 8 | 5839 | OWO WAT V 397 | 50.176 | 56.086 | 14.851 | 1.00 | 28.75 | 8 |
| 5799 | OWO WAT V 356 | 23.545 | 83.502 | 8.615 | 1.00 | 27.06 | 8 | 5840 | OWO WAT V 398 | 14.115 | 57.834 | 59.211 | 1.00 | 27.83 | 8 |
| 5800 | OWO WAT V 357 | 22.122 | 49.913 | 14.384 | 1.00 | 27.06 | 8 | 5841 | OWO WAT V 399 | 38.189 | 49.702 | 11.383 | 1.00 | 29.29 | 8 |
| 5801 | OWO WAT V 358 | 6.833 | 52.668 | 34.000 | 1.00 | 27.79 | 8 | 5842 | OWO WAT V 400 | 3.241 | 100.941 | 39.033 | 1.00 | 28.47 | 8 |
| 5802 | OWO WAT V 359 | 30.479 | 47.598 | 56.666 | 1.00 | 27.66 | 8 | 5843 | OWO WAT V 401 | 44.298 | 73.510 | 63.099 | 1.00 | 28.91 | 8 |
| 5803 | OWO WAT V 360 | 33.166 | 42.826 | 19.802 | 1.00 | 27.33 | 8 | 5844 | OWO WAT V 402 | 7.061 | 75.135 | 47.544 | 1.00 | 28.59 | 8 |
| 5804 | OWO WAT V 361 | 24.029 | 55.851 | 13.947 | 1.00 | 27.33 | 8 | 5845 | OWO WAT V 403 | 5.477 | 86.910 | 42.452 | 1.00 | 29.56 | 8 |
| 5805 | OWO WAT V 362 | 39.488 | 85.709 | 20.632 | 1.00 | 27.01 | 8 | 5846 | OWO WAT V 404 | 25.564 | 72.515 | 56.246 | 1.00 | 29.09 | 8 |
| 5806 | OWO WAT V 363 | 2.130 | 49.916 | 43.049 | 1.00 | 27.26 | 8 | 5847 | OWO WAT V 405 | 25.075 | 41.160 | 32.189 | 1.00 | 29.20 | 8 |
| 5807 | OWO WAT V 364 | 35.616 | 41.373 | 27.626 | 1.00 | 27.13 | 8 | 5848 | OWO WAT V 406 | 2.074 | 56.387 | 58.854 | 1.00 | 28.86 | 8 |
| | OWO WAT V 365 | 50.664 | 58.560 | 41.450 | 1.00 | 26.59 | 8 | 5849 | OWO WAT V 407 | 47.163 | 58.038 | 33.355 | 1.00 | 28.76 | 8 |

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|------|---------------|--------|---------|--------|------------|---|------|---------------|--------|---------|--------|------------|---|
| 5850 | OWO WAT V 408 | 27.438 | 44.407 | 21.116 | 1.00 28.21 | 8 | 5892 | OWO WAT V 450 | 8.486 | 84.645 | 16.251 | 1.00 30.46 | 8 |
| 5851 | OWO WAT V 409 | 32.690 | 89.765 | 34.445 | 1.00 29.13 | 8 | 5893 | OWO WAT V 451 | 17.712 | 70.200 | 52.856 | 1.00 31.30 | 8 |
| 5852 | OWO WAT V 410 | 8.726 | 56.984 | 33.875 | 1.00 28.81 | 8 | 5894 | OWO WAT V 452 | 45.187 | 54.640 | 9.218 | 1.00 30.47 | 8 |
| 5853 | OWO WAT V 411 | -2.765 | 74.847 | 45.763 | 1.00 28.58 | 8 | 5895 | OWO WAT V 453 | 23.220 | 65.098 | 2.001 | 1.00 30.15 | 8 |
| 5854 | OWO WAT V 412 | 9.880 | 76.028 | 48.593 | 1.00 29.43 | 8 | 5896 | OWO WAT V 454 | 43.353 | 48.993 | 23.792 | 1.00 30.21 | 8 |
| 5855 | OWO WAT V 413 | 18.587 | 55.405 | 41.191 | 1.00 28.66 | 8 | 5897 | OWO WAT V 455 | 0.241 | 76.716 | 42.809 | 1.00 30.43 | 8 |
| 5856 | OWO WAT V 414 | 0.831 | 95.595 | 23.928 | 1.00 28.90 | 8 | 5898 | OWO WAT V 456 | 38.954 | 90.362 | 25.885 | 1.00 31.19 | 8 |
| 5857 | OWO WAT V 415 | 18.167 | 58.042 | 65.360 | 1.00 28.57 | 8 | 5899 | OWO WAT V 457 | 8.998 | 51.618 | 42.193 | 1.00 30.65 | 8 |
| 5858 | OWO WAT V 416 | 42.814 | 47.661 | 27.620 | 1.00 29.34 | 8 | 5900 | OWO WAT V 458 | 47.484 | 70.509 | 20.484 | 1.00 30.75 | 8 |
| 5859 | OWO WAT V 417 | 19.226 | 89.316 | 19.020 | 1.00 29.13 | 8 | 5901 | OWO WAT V 459 | 26.632 | 83.732 | 7.006 | 1.00 30.86 | 8 |
| 5860 | OWO WAT V 418 | 17.933 | 82.283 | 11.952 | 1.00 28.48 | 8 | 5902 | OWO WAT V 460 | 27.887 | 84.031 | 46.702 | 1.00 31.16 | 8 |
| 5861 | OWO WAT V 419 | 44.723 | 79.313 | 13.493 | 1.00 30.12 | 8 | 5903 | OWO WAT V 461 | 10.456 | 52.659 | 39.931 | 1.00 31.37 | 8 |
| 5862 | OWO WAT V 420 | 34.399 | 78.316 | 0.819 | 1.00 29.81 | 8 | 5904 | OWO WAT V 462 | 25.474 | 53.247 | 11.551 | 1.00 31.54 | 8 |
| 5863 | OWO WAT V 421 | 28.282 | 72.460 | 57.888 | 1.00 29.12 | 8 | 5905 | OWO WAT V 463 | 21.666 | 48.674 | 41.178 | 1.00 31.71 | 8 |
| 5864 | OWO WAT V 422 | 50.448 | 63.547 | 18.793 | 1.00 29.31 | 8 | 5906 | OWO WAT V 464 | 51.799 | 63.643 | 37.234 | 1.00 30.69 | 8 |
| 5865 | OWO WAT V 423 | 43.033 | 55.323 | 65.913 | 1.00 29.32 | 8 | 5907 | OWO WAT V 465 | 17.686 | 48.668 | 36.134 | 1.00 31.38 | 8 |
| 5866 | OWO WAT V 424 | 45.865 | 51.168 | 51.498 | 1.00 29.29 | 8 | 5908 | OWO WAT V 466 | 47.081 | 52.951 | 49.717 | 1.00 30.51 | 8 |
| 5867 | OWO WAT V 425 | 12.844 | 59.751 | 19.386 | 1.00 29.45 | 8 | 5909 | OWO WAT V 467 | 15.593 | 93.203 | 42.768 | 1.00 30.90 | 8 |
| 5868 | OWO WAT V 426 | -3.707 | 82.697 | 22.959 | 1.00 29.58 | 8 | 5910 | OWO WAT V 468 | 36.480 | 80.071 | 53.771 | 1.00 30.56 | 8 |
| 5869 | OWO WAT V 427 | 28.989 | 45.171 | 18.941 | 1.00 29.97 | 8 | 5911 | OWO WAT V 469 | 42.137 | 47.781 | 14.882 | 1.00 31.85 | 8 |
| 5870 | OWO WAT V 428 | 14.689 | 65.149 | 11.472 | 1.00 29.76 | 8 | 5912 | OWO WAT V 470 | 22.333 | 61.351 | 70.096 | 1.00 31.36 | 8 |
| 5871 | OWO WAT V 429 | 49.962 | 74.061 | 53.235 | 1.00 29.59 | 8 | 5913 | OWO WAT V 471 | 40.228 | 72.527 | 72.095 | 1.00 31.17 | 8 |
| 5872 | OWO WAT V 430 | 26.674 | 46.428 | 17.647 | 1.00 29.59 | 8 | 5914 | OWO WAT V 472 | 1.666 | 74.527 | 48.132 | 1.00 31.28 | 8 |
| 5873 | OWO WAT V 431 | 32.017 | 64.281 | 73.846 | 1.00 29.67 | 8 | 5915 | OWO WAT V 473 | 14.531 | 66.936 | 59.718 | 1.00 31.26 | 8 |
| 5874 | OWO WAT V 432 | -1.685 | 89.735 | 36.396 | 1.00 29.42 | 8 | 5916 | OWO WAT V 474 | 21.000 | 68.421 | 1.879 | 1.00 31.59 | 8 |
| 5875 | OWO WAT V 433 | 35.326 | 90.671 | 32.858 | 1.00 30.08 | 8 | 5917 | OWO WAT V 475 | 37.163 | 82.170 | 41.385 | 1.00 31.32 | 8 |
| 5876 | OWO WAT V 434 | -5.217 | 86.519 | 22.737 | 1.00 30.64 | 8 | 5918 | OWO WAT V 476 | 26.307 | 62.094 | 4.445 | 1.00 31.75 | 8 |
| 5877 | OWO WAT V 435 | 22.655 | 40.619 | 31.468 | 1.00 30.18 | 8 | 5919 | OWO WAT V 477 | 51.579 | 61.409 | 40.641 | 1.00 31.25 | 8 |
| 5878 | OWO WAT V 436 | 9.970 | 66.686 | 21.940 | 1.00 30.16 | 8 | 5920 | OWO WAT V 478 | 41.761 | 64.533 | 7.578 | 1.00 31.59 | 8 |
| 5879 | OWO WAT V 437 | 22.156 | 103.267 | 41.579 | 1.00 28.97 | 8 | 5921 | OWO WAT V 479 | -7.353 | 65.632 | 35.219 | 1.00 31.13 | 8 |
| 5880 | OWO WAT V 438 | 40.919 | 45.553 | 23.996 | 1.00 30.13 | 8 | 5922 | OWO WAT V 480 | 16.514 | 82.720 | 36.237 | 1.00 31.25 | 8 |
| 5881 | OWO WAT V 439 | 24.378 | 42.994 | 18.498 | 1.00 30.25 | 8 | 5923 | OWO WAT V 481 | 23.770 | 75.891 | 54.586 | 1.00 31.53 | 8 |
| 5882 | OWO WAT V 440 | 27.456 | 90.485 | 38.760 | 1.00 29.87 | 8 | 5924 | OWO WAT V 482 | 50.377 | 68.458 | 56.245 | 1.00 31.72 | 8 |
| 5883 | OWO WAT V 441 | 41.628 | 78.372 | 57.406 | 1.00 30.24 | 8 | 5925 | OWO WAT V 483 | 15.979 | 105.053 | 38.501 | 1.00 30.98 | 8 |
| 5884 | OWO WAT V 442 | 10.162 | 67.365 | 58.879 | 1.00 30.51 | 8 | 5926 | OWO WAT V 484 | 27.194 | 93.867 | 31.829 | 1.00 31.85 | 8 |
| 5885 | OWO WAT V 443 | 7.899 | 70.258 | 55.642 | 1.00 29.98 | 8 | 5927 | OWO WAT V 485 | 39.487 | 68.664 | 5.438 | 1.00 31.02 | 8 |
| 5886 | OWO WAT V 444 | 7.439 | 62.721 | 58.664 | 1.00 30.04 | 8 | 5928 | OWO WAT V 486 | 30.446 | 58.438 | 75.573 | 1.00 31.49 | 8 |
| 5887 | OWO WAT V 445 | 30.182 | 60.296 | 5.170 | 1.00 30.62 | 8 | 5929 | OWO WAT V 487 | -2.258 | 85.349 | 34.418 | 1.00 31.74 | 8 |
| 5888 | OWO WAT V 446 | 36.835 | 87.065 | 16.010 | 1.00 30.22 | 8 | 5930 | OWO WAT V 488 | 46.873 | 56.769 | 65.770 | 1.00 31.57 | 8 |
| 5889 | OWO WAT V 447 | 48.154 | 58.076 | 55.789 | 1.00 30.39 | 8 | 5931 | OWO WAT V 489 | 18.407 | 47.617 | 19.229 | 1.00 31.61 | 8 |
| 5890 | OWO WAT V 448 | 9.079 | 102.838 | 38.708 | 1.00 30.45 | 8 | 5932 | OWO WAT V 490 | 2.500 | 78.686 | 43.392 | 1.00 31.62 | 8 |
| 5891 | OWO WAT V 449 | 31.488 | 67.009 | 5.903 | 1.00 30.35 | 8 | 5933 | OWO WAT V 491 | 7.727 | 97.913 | 42.497 | 1.00 32.36 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 5934 | OWO WAT V 492 | -5.430 | 71.658 | 30.991 | 1.00 | 32.45 | 8 | 5976 | OWO WAT V 534 | 35.615 | 48.266 | 53.410 | 1.00 | 33.74 | 8 |
| 5935 | OWO WAT V 493 | 47.547 | 72.958 | 21.222 | 1.00 | 31.57 | 8 | 5977 | OWO WAT V 535 | 50.581 | 54.379 | 41.752 | 1.00 | 32.75 | 8 |
| 5936 | OWO WAT V 494 | 9.955 | 91.961 | 24.393 | 1.00 | 32.43 | 8 | 5978 | OWO WAT V 536 | 34.738 | 50.213 | 7.372 | 1.00 | 33.68 | 8 |
| 5937 | OWO WAT V 495 | 12.996 | 52.420 | 46.232 | 1.00 | 31.76 | 8 | 5979 | OWO WAT V 537 | 42.324 | 79.266 | 54.340 | 1.00 | 32.72 | 8 |
| 5938 | OWO WAT V 496 | 7.952 | 65.594 | 58.841 | 1.00 | 32.02 | 8 | 5980 | OWO WAT V 538 | 16.132 | 78.441 | 8.864 | 1.00 | 33.64 | 8 |
| 5939 | OWO WAT V 497 | 37.204 | 88.789 | 33.415 | 1.00 | 31.57 | 8 | 5981 | OWO WAT V 539 | 20.256 | 45.911 | 20.702 | 1.00 | 33.89 | 8 |
| 5940 | OWO WAT V 498 | 36.857 | 41.938 | 29.865 | 1.00 | 32.38 | 8 | 5982 | OWO WAT V 540 | 37.253 | 43.882 | 46.170 | 1.00 | 33.73 | 8 |
| 5941 | OWO WAT V 499 | 7.220 | 51.844 | 54.727 | 1.00 | 32.32 | 8 | 5983 | OWO WAT V 541 | 31.158 | 88.960 | 12.651 | 1.00 | 34.15 | 8 |
| 5942 | OWO WAT V 500 | 16.110 | 76.377 | 49.777 | 1.00 | 32.31 | 8 | 5984 | OWO WAT V 542 | 2.885 | 65.252 | 30.182 | 1.00 | 33.66 | 8 |
| 5943 | OWO WAT V 501 | 24.511 | 47.736 | 42.135 | 1.00 | 32.37 | 8 | 5985 | OWO WAT V 543 | 24.093 | 72.008 | 54.068 | 1.00 | 33.53 | 8 |
| 5944 | OWO WAT V 502 | 22.783 | 46.357 | 48.051 | 1.00 | 32.64 | 8 | 5986 | OWO WAT V 544 | -4.660 | 58.902 | 52.534 | 1.00 | 34.13 | 8 |
| 5945 | OWO WAT V 503 | 27.138 | 60.897 | 7.569 | 1.00 | 32.20 | 8 | 5987 | OWO WAT V 545 | 20.523 | 52.571 | 71.335 | 1.00 | 34.29 | 8 |
| 5946 | OWO WAT V 504 | 47.227 | 50.290 | 36.850 | 1.00 | 32.13 | 8 | 5988 | OWO WAT V 546 | 50.389 | 70.373 | 43.120 | 1.00 | 34.05 | 8 |
| 5947 | OWO WAT V 505 | 6.733 | 67.493 | 23.991 | 1.00 | 32.68 | 8 | 5989 | OWO WAT V 547 | -1.784 | 74.917 | 34.717 | 1.00 | 34.27 | 8 |
| 5948 | OWO WAT V 506 | 16.514 | 70.176 | 56.941 | 1.00 | 32.03 | 8 | 5990 | OWO WAT V 548 | 25.051 | 100.468 | 31.517 | 1.00 | 33.73 | 8 |
| 5949 | OWO WAT V 507 | 43.175 | 79.662 | 8.514 | 1.00 | 31.76 | 8 | 5991 | OWO WAT V 549 | 21.989 | 83.148 | 46.194 | 1.00 | 34.71 | 8 |
| 5950 | OWO WAT V 508 | -3.757 | 80.394 | 22.899 | 1.00 | 32.62 | 8 | 5992 | OWO WAT V 550 | 47.521 | 62.364 | 11.718 | 1.00 | 34.05 | 8 |
| 5951 | OWO WAT V 509 | 10.932 | 85.936 | 45.262 | 1.00 | 32.65 | 8 | 5993 | OWO WAT V 551 | 52.236 | 59.305 | 62.786 | 1.00 | 33.21 | 8 |
| 5952 | OWO WAT V 510 | 3.455 | 97.650 | 41.755 | 1.00 | 32.31 | 8 | 5994 | OWO WAT V 552 | 40.232 | 80.510 | 16.448 | 1.00 | 34.62 | 8 |
| 5953 | OWO WAT V 511 | 33.419 | 50.551 | 69.455 | 1.00 | 32.14 | 8 | 5995 | OWO WAT V 553 | 46.253 | 56.949 | 70.930 | 1.00 | 33.53 | 8 |
| 5954 | OWO WAT V 512 | 4.069 | 99.962 | 23.550 | 1.00 | 33.21 | 8 | 5996 | OWO WAT V 554 | 47.895 | 53.053 | 37.454 | 1.00 | 33.41 | 8 |
| 5955 | OWO WAT V 513 | -7.206 | 65.717 | 61.406 | 1.00 | 33.20 | 8 | 5997 | OWO WAT V 555 | 13.358 | 71.030 | 49.662 | 1.00 | 34.43 | 8 |
| 5956 | OWO WAT V 514 | 53.785 | 80.262 | 41.406 | 1.00 | 33.37 | 8 | 5998 | OWO WAT V 556 | -0.137 | 73.990 | 26.087 | 1.00 | 34.05 | 8 |
| 5957 | OWO WAT V 515 | 16.599 | 87.045 | 17.346 | 1.00 | 32.99 | 8 | 5999 | OWO WAT V 557 | 43.973 | 74.382 | 6.399 | 1.00 | 34.44 | 8 |
| 5958 | OWO WAT V 516 | 47.349 | 54.074 | 30.752 | 1.00 | 32.14 | 8 | 6000 | OWO WAT V 558 | 35.593 | 60.367 | 77.022 | 1.00 | 33.63 | 8 |
| 5959 | OWO WAT V 517 | 7.038 | 85.163 | 42.409 | 1.00 | 32.78 | 8 | 6001 | OWO WAT V 559 | 6.112 | 83.592 | 41.192 | 1.00 | 34.97 | 8 |
| 5960 | OWO WAT V 518 | 16.879 | 50.503 | 27.538 | 1.00 | 32.69 | 8 | 6002 | OWO WAT V 560 | 38.614 | 41.425 | 25.492 | 1.00 | 34.42 | 8 |
| 5961 | OWO WAT V 519 | 30.838 | 91.776 | 22.385 | 1.00 | 33.06 | 8 | 6003 | OWO WAT V 561 | 34.074 | 88.144 | 12.960 | 1.00 | 34.41 | 8 |
| 5962 | OWO WAT V 520 | 33.882 | 41.296 | 32.218 | 1.00 | 34.59 | 8 | 6004 | OWO WAT V 562 | 40.114 | 63.213 | 5.786 | 1.00 | 34.56 | 8 |
| 5963 | OWO WAT V 521 | 53.502 | 60.512 | 23.358 | 1.00 | 32.27 | 8 | 6005 | OWO WAT V 563 | -0.202 | 64.215 | 60.019 | 1.00 | 34.60 | 8 |
| 5964 | OWO WAT V 522 | 41.841 | 73.003 | 34.316 | 1.00 | 33.63 | 8 | 6006 | OWO WAT V 564 | 4.614 | 92.264 | 20.329 | 1.00 | 33.82 | 8 |
| 5965 | OWO WAT V 523 | 18.807 | 69.394 | 5.371 | 1.00 | 32.65 | 8 | 6007 | OWO WAT V 565 | 15.212 | 50.738 | 32.687 | 1.00 | 34.54 | 8 |
| 5966 | OWO WAT V 524 | 0.567 | 102.365 | 27.670 | 1.00 | 32.87 | 8 | 6008 | OWO WAT V 566 | 13.018 | 70.753 | 53.378 | 1.00 | 35.00 | 8 |
| 5967 | OWO WAT V 525 | 28.899 | 48.822 | 64.451 | 1.00 | 32.62 | 8 | 6009 | OWO WAT V 567 | 37.836 | 57.700 | 75.968 | 1.00 | 33.91 | 8 |
| 5968 | OWO WAT V 526 | 42.766 | 46.627 | 21.339 | 1.00 | 33.04 | 8 | 6010 | OWO WAT V 568 | 18.054 | 71.354 | 7.047 | 1.00 | 34.28 | 8 |
| 5969 | OWO WAT V 527 | 18.159 | 66.472 | 60.034 | 1.00 | 33.02 | 8 | 6011 | OWO WAT V 569 | 20.435 | 57.091 | 12.782 | 1.00 | 34.06 | 8 |
| 5970 | OWO WAT V 528 | 22.385 | 49.518 | 59.427 | 1.00 | 33.48 | 8 | 6012 | OWO WAT V 570 | -1.113 | 72.836 | 30.802 | 1.00 | 34.18 | 8 |
| 5971 | OWO WAT V 529 | 14.542 | 53.899 | 35.438 | 1.00 | 32.40 | 8 | 6013 | OWO WAT V 571 | 45.394 | 47.985 | 15.576 | 1.00 | 34.25 | 8 |
| 5972 | OWO WAT V 530 | 0.923 | 81.260 | 18.821 | 1.00 | 33.19 | 8 | 6014 | OWO WAT V 572 | 18.083 | 105.524 | 25.739 | 1.00 | 35.26 | 8 |
| 5973 | OWO WAT V 531 | 35.980 | 91.602 | 25.073 | 1.00 | 32.89 | 8 | 6015 | OWO WAT V 573 | 42.363 | 51.035 | 61.868 | 1.00 | 34.64 | 8 |
| 5974 | OWO WAT V 532 | 40.667 | 67.024 | 71.313 | 1.00 | 32.79 | 8 | 6016 | OWO WAT V 574 | 3.332 | 65.717 | 27.045 | 1.00 | 35.54 | 8 |
| 5975 | OWO WAT V 533 | 8.626 | 61.294 | 60.713 | 1.00 | 32.69 | 8 | 6017 | OWO WAT V 575 | 0.099 | 70.672 | 51.291 | 1.00 | 34.72 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 6018 | OWO WAT V 576 | 0.045 | 61.496 | 31.457 | 1.00 | 35.51 | 8 | 6060 | OWO WAT V 618 | 40.907 | 80.214 | 52.034 | 1.00 | 37.09 | 8 |
| 6019 | OWO WAT V 577 | 46.395 | 53.881 | 61.040 | 1.00 | 34.53 | 8 | 6061 | OWO WAT V 619 | 47.006 | 72.793 | 58.223 | 1.00 | 36.47 | 8 |
| 6020 | OWO WAT V 578 | 52.136 | 68.150 | 59.956 | 1.00 | 35.10 | 8 | 6062 | OWO WAT V 620 | 20.221 | 90.473 | 42.499 | 1.00 | 36.27 | 8 |
| 6021 | OWO WAT V 579 | 19.009 | 41.546 | 26.130 | 1.00 | 33.65 | 8 | 6063 | OWO WAT V 621 | 4.100 | 73.674 | 21.447 | 1.00 | 36.94 | 8 |
| 6022 | OWO WAT V 580 | 34.720 | 74.712 | 71.942 | 1.00 | 34.54 | 8 | 6064 | OWO WAT V 622 | 8.503 | 104.300 | 35.973 | 1.00 | 36.81 | 8 |
| 6023 | OWO WAT V 581 | 37.259 | 73.783 | 73.743 | 1.00 | 35.82 | 8 | 6065 | OWO WAT V 623 | 30.691 | 78.729 | 57.692 | 1.00 | 35.94 | 8 |
| 6024 | OWO WAT V 582 | 27.833 | 55.518 | 10.945 | 1.00 | 34.54 | 8 | 6066 | OWO WAT V 624 | -3.070 | 94.866 | 30.332 | 1.00 | 36.58 | 8 |
| 6025 | OWO WAT V 583 | 46.309 | 60.566 | 10.060 | 1.00 | 35.04 | 8 | 6067 | OWO WAT V 625 | 46.455 | 79.736 | 18.637 | 1.00 | 35.97 | 8 |
| 6026 | OWO WAT V 584 | 10.952 | 63.329 | 18.773 | 1.00 | 34.23 | 8 | 6068 | OWO WAT V 626 | 46.537 | 55.701 | 59.420 | 1.00 | 37.10 | 8 |
| 6027 | OWO WAT V 585 | -1.056 | 54.481 | 35.620 | 1.00 | 34.65 | 8 | 6069 | OWO WAT V 627 | 43.765 | 47.227 | 50.091 | 1.00 | 37.02 | 8 |
| 6028 | OWO WAT V 586 | -4.178 | 63.600 | 36.602 | 1.00 | 35.48 | 8 | 6070 | OWO WAT V 628 | -0.451 | 52.302 | 37.499 | 1.00 | 36.00 | 8 |
| 6029 | OWO WAT V 587 | 4.690 | 96.750 | 20.660 | 1.00 | 34.69 | 8 | 6071 | OWO WAT V 629 | 47.301 | 50.088 | 41.392 | 1.00 | 37.12 | 8 |
| 6030 | OWO WAT V 588 | 8.484 | 73.376 | 50.572 | 1.00 | 35.07 | 8 | 6072 | OWO WAT V 630 | 37.956 | 80.815 | 13.060 | 1.00 | 37.94 | 8 |
| 6031 | OWO WAT V 589 | 44.017 | 50.506 | 11.023 | 1.00 | 35.68 | 8 | 6073 | OWO WAT V 631 | 17.138 | 62.973 | 7.515 | 1.00 | 37.42 | 8 |
| 6032 | OWO WAT V 590 | 3.744 | 50.549 | 36.911 | 1.00 | 35.69 | 8 | 6074 | OWO WAT V 632 | 13.837 | 57.372 | 18.395 | 1.00 | 36.82 | 8 |
| 6033 | OWO WAT V 591 | 49.672 | 55.539 | 26.394 | 1.00 | 35.74 | 8 | 6075 | OWO WAT V 633 | 41.756 | 55.821 | 70.896 | 1.00 | 36.92 | 8 |
| 6034 | OWO WAT V 592 | 27.932 | 93.666 | 25.261 | 1.00 | 35.64 | 8 | 6076 | OWO WAT V 634 | 25.077 | 93.998 | 28.706 | 1.00 | 36.97 | 8 |
| 6035 | OWO WAT V 593 | 22.451 | 73.996 | 54.266 | 1.00 | 35.51 | 8 | 6077 | OWO WAT V 635 | 47.608 | 54.704 | 64.130 | 1.00 | 37.13 | 8 |
| 6036 | OWO WAT V 594 | 33.048 | 48.697 | 67.743 | 1.00 | 35.66 | 8 | 6078 | OWO WAT V 636 | 6.911 | 105.878 | 25.141 | 1.00 | 36.23 | 8 |
| 6037 | OWO WAT V 595 | 12.820 | 101.046 | 44.339 | 1.00 | 36.16 | 8 | 6079 | OWO WAT V 637 | 42.682 | 67.557 | 69.041 | 1.00 | 36.92 | 8 |
| 6038 | OWO WAT V 596 | 51.198 | 69.586 | 53.643 | 1.00 | 35.14 | 8 | 6080 | OWO WAT V 638 | 15.363 | 88.594 | 48.034 | 1.00 | 37.42 | 8 |
| 6039 | OWO WAT V 597 | 29.662 | 79.574 | 54.942 | 1.00 | 35.66 | 8 | 6081 | OWO WAT V 639 | 33.890 | 42.321 | 17.015 | 1.00 | 37.23 | 8 |
| 6040 | OWO WAT V 598 | 32.247 | 80.128 | 52.116 | 1.00 | 36.54 | 8 | 6082 | OWO WAT V 640 | 9.736 | 84.033 | 43.853 | 1.00 | 36.17 | 8 |
| 6041 | OWO WAT V 599 | 6.142 | 51.551 | 37.685 | 1.00 | 35.34 | 8 | 6083 | OWO WAT V 641 | 10.886 | 51.035 | 46.103 | 1.00 | 37.66 | 8 |
| 6042 | OWO WAT V 600 | 5.622 | 70.631 | 22.637 | 1.00 | 35.66 | 8 | 6084 | OWO WAT V 642 | 27.929 | 72.978 | 70.610 | 1.00 | 37.35 | 8 |
| 6043 | OWO WAT V 601 | 22.365 | 48.081 | 48.242 | 1.00 | 36.08 | 8 | 6085 | OWO WAT V 643 | 1.233 | 69.664 | 25.786 | 1.00 | 37.56 | 8 |
| 6044 | OWO WAT V 602 | 8.288 | 81.332 | 15.641 | 1.00 | 35.59 | 8 | 6086 | OWO WAT V 644 | 15.151 | 107.231 | 33.216 | 1.00 | 36.50 | 8 |
| 6045 | OWO WAT V 603 | 10.941 | 74.805 | 15.117 | 1.00 | 35.60 | 8 | 6087 | OWO WAT V 645 | 25.823 | 98.361 | 30.305 | 1.00 | 36.65 | 8 |
| 6046 | OWO WAT V 604 | 35.796 | 73.953 | 1.142 | 1.00 | 35.09 | 8 | 6088 | OWO WAT V 646 | 34.857 | 84.394 | 12.899 | 1.00 | 36.71 | 8 |
| 6047 | OWO WAT V 605 | 38.777 | 85.286 | 9.309 | 1.00 | 36.46 | 8 | 6089 | OWO WAT V 647 | 20.425 | 52.936 | 41.877 | 1.00 | 36.99 | 8 |
| 6048 | OWO WAT V 606 | 20.560 | 52.963 | 75.539 | 1.00 | 37.03 | 8 | 6090 | OWO WAT V 648 | 26.575 | 49.377 | 65.800 | 1.00 | 37.37 | 8 |
| 6049 | OWO WAT V 607 | -3.377 | 66.230 | 32.749 | 1.00 | 35.54 | 8 | 6091 | OWO WAT V 649 | 31.193 | 44.914 | 15.071 | 1.00 | 36.96 | 8 |
| 6050 | OWO WAT V 608 | 40.087 | 44.107 | 14.031 | 1.00 | 36.33 | 8 | 6092 | OWO WAT V 650 | 10.578 | 49.772 | 48.688 | 1.00 | 36.01 | 8 |
| 6051 | OWO WAT V 609 | -1.635 | 86.958 | 36.864 | 1.00 | 35.23 | 8 | 6093 | OWO WAT V 651 | 18.128 | 51.717 | 38.409 | 1.00 | 37.57 | 8 |
| 6052 | OWO WAT V 610 | 48.364 | 69.799 | 29.088 | 1.00 | 35.08 | 8 | 6094 | OWO WAT V 652 | 45.424 | 54.692 | 56.844 | 1.00 | 37.37 | 8 |
| 6053 | OWO WAT V 611 | 18.383 | 50.939 | 35.706 | 1.00 | 36.23 | 8 | 6095 | OWO WAT V 653 | 28.011 | 90.646 | 18.192 | 1.00 | 37.91 | 8 |
| 6054 | OWO WAT V 612 | 18.334 | 58.135 | 13.735 | 1.00 | 37.22 | 8 | 6096 | OWO WAT V 654 | 47.536 | 55.043 | 51.941 | 1.00 | 36.73 | 8 |
| 6055 | OWO WAT V 613 | 16.341 | 55.369 | 50.997 | 1.00 | 35.78 | 8 | 6097 | OWO WAT V 655 | 24.853 | 98.451 | 32.915 | 1.00 | 37.70 | 8 |
| 6056 | OWO WAT V 614 | 28.580 | 52.384 | 12.139 | 1.00 | 36.07 | 8 | 6098 | OWO WAT V 656 | 27.088 | 98.198 | 26.870 | 1.00 | 38.56 | 8 |
| 6057 | OWO WAT V 615 | 23.108 | 103.615 | 38.927 | 1.00 | 36.81 | 8 | 6099 | OWO WAT V 657 | 33.663 | 49.796 | 11.597 | 1.00 | 37.19 | 8 |
| 6058 | OWO WAT V 616 | 12.325 | 79.803 | 46.301 | 1.00 | 35.61 | 8 | 6100 | OWO WAT V 658 | 16.309 | 55.242 | 45.035 | 1.00 | 37.83 | 8 |
| 6059 | OWO WAT V 617 | 21.280 | 67.375 | 64.153 | 1.00 | 36.55 | 8 | 6101 | OWO WAT V 659 | 20.804 | 43.210 | 25.195 | 1.00 | 37.72 | 8 |

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| 6102 | OWO WAT V 660 | 23.932 | 65.246 | 70.893 | 1.00 | 37.09 | 8 | 6144 | OWO WAT V 702 | 36.514 | 82.654 | 34.129 | 1.00 | 38.10 | 8 |
| 6103 | OWO WAT V 661 | 0.664 | 53.286 | 53.271 | 1.00 | 38.36 | 8 | 6145 | OWO WAT V 703 | 43.559 | 50.161 | 59.718 | 1.00 | 39.15 | 8 |
| 6104 | OWO WAT V 662 | 40.187 | 84.151 | 18.538 | 1.00 | 38.05 | 8 | 6146 | OWO WAT V 704 | 41.881 | 70.064 | 7.497 | 1.00 | 39.49 | 8 |
| 6105 | OWO WAT V 663 | 44.129 | 77.826 | 7.095 | 1.00 | 38.36 | 8 | 6147 | OWO WAT V 705 | 12.039 | 106.892 | 30.442 | 1.00 | 39.69 | 8 |
| 6106 | OWO WAT V 664 | 5.654 | 103.176 | 36.651 | 1.00 | 38.12 | 8 | 6148 | OWO WAT V 706 | 25.673 | 81.581 | 52.252 | 1.00 | 39.17 | 8 |
| 6107 | OWO WAT V 665 | -2.551 | 55.092 | 37.581 | 1.00 | 39.63 | 8 | 6149 | OWO WAT V 707 | 46.855 | 74.915 | 26.181 | 1.00 | 40.35 | 8 |
| 6108 | OWO WAT V 666 | 48.102 | 56.702 | 13.267 | 1.00 | 37.64 | 8 | 6150 | OWO WAT V 708 | 21.077 | 93.052 | 39.231 | 1.00 | 39.44 | 8 |
| 6109 | OWO WAT V 667 | 27.824 | 90.475 | 15.555 | 1.00 | 36.41 | 8 | 6151 | OWO WAT V 709 | 28.621 | 62.328 | 5.470 | 1.00 | 38.56 | 8 |
| 6110 | OWO WAT V 668 | 38.699 | 49.812 | 63.112 | 1.00 | 37.80 | 8 | 6152 | OWO WAT V 710 | -3.607 | 57.742 | 54.506 | 1.00 | 38.82 | 8 |
| 6111 | OWO WAT V 669 | -2.199 | 54.401 | 53.588 | 1.00 | 39.21 | 8 | 6153 | OWO WAT V 711 | 25.913 | 41.714 | 29.843 | 1.00 | 38.94 | 8 |
| 6112 | OWO WAT V 670 | 19.006 | 53.240 | 47.228 | 1.00 | 38.93 | 8 | 6154 | OWO WAT V 712 | 21.385 | 95.763 | 42.160 | 1.00 | 39.85 | 8 |
| 6113 | OWO WAT V 671 | 46.897 | 48.817 | 19.829 | 1.00 | 39.11 | 8 | 6155 | OWO WAT V 713 | 39.666 | 46.565 | 56.093 | 1.00 | 40.16 | 8 |
| 6114 | OWO WAT V 672 | 42.301 | 48.935 | 12.664 | 1.00 | 37.43 | 8 | 6156 | OWO WAT V 714 | 33.043 | 47.398 | 12.747 | 1.00 | 38.56 | 8 |
| 6115 | OWO WAT V 673 | 16.098 | 53.972 | 53.322 | 1.00 | 38.55 | 8 | 6157 | OWO WAT V 715 | 3.335 | 48.480 | 47.523 | 1.00 | 40.24 | 8 |
| 6116 | OWO WAT V 674 | 16.992 | 66.360 | 61.965 | 1.00 | 40.47 | 8 | 6158 | OWO WAT V 716 | -5.954 | 59.355 | 43.289 | 1.00 | 39.30 | 8 |
| 6117 | OWO WAT V 675 | 17.396 | 84.259 | 14.592 | 1.00 | 37.45 | 8 | 6159 | OWO WAT V 717 | -2.633 | 70.380 | 52.100 | 1.00 | 39.49 | 8 |
| 6118 | OWO WAT V 676 | 48.023 | 70.300 | 38.414 | 1.00 | 38.28 | 8 | 6160 | OWO WAT V 718 | 14.943 | 51.881 | 28.927 | 1.00 | 41.17 | 8 |
| 6119 | OWO WAT V 677 | 21.061 | 60.355 | 72.008 | 1.00 | 38.68 | 8 | 6161 | OWO WAT V 719 | 30.665 | 55.789 | 76.270 | 1.00 | 36.29 | 8 |
| 6120 | OWO WAT V 678 | 25.412 | 45.777 | 15.102 | 1.00 | 40.05 | 8 | 6162 | OWO WAT V 720 | 38.153 | 41.243 | 44.336 | 1.00 | 39.61 | 8 |
| 6121 | OWO WAT V 679 | 43.705 | 73.272 | 1.624 | 1.00 | 38.78 | 8 | 6163 | OWO WAT V 721 | 42.857 | 72.924 | 4.760 | 1.00 | 39.33 | 8 |
| 6122 | OWO WAT V 680 | 17.379 | 67.334 | 7.173 | 1.00 | 38.98 | 8 | 6164 | OWO WAT V 722 | 42.983 | 45.506 | 30.086 | 1.00 | 39.35 | 8 |
| 6123 | OWO WAT V 681 | 19.500 | 72.583 | 5.113 | 1.00 | 41.12 | 8 | 6165 | OWO WAT V 723 | 8.541 | 68.671 | 15.477 | 1.00 | 40.10 | 8 |
| 6124 | OWO WAT V 682 | 27.135 | 53.269 | 75.096 | 1.00 | 38.74 | 8 | 6166 | OWO WAT V 724 | 3.357 | 68.745 | 24.682 | 1.00 | 39.21 | 8 |
| 6125 | OWO WAT V 683 | 43.871 | 76.670 | 2.397 | 1.00 | 38.42 | 8 | 6167 | OWO WAT V 725 | 32.096 | 74.899 | 2.155 | 1.00 | 38.68 | 8 |
| 6126 | OWO WAT V 684 | 32.690 | 47.277 | 60.342 | 1.00 | 38.23 | 8 | 6168 | OWO WAT V 726 | -3.316 | 99.677 | 31.930 | 1.00 | 40.29 | 8 |
| 6127 | OWO WAT V 685 | 38.889 | 50.643 | 67.387 | 1.00 | 38.05 | 8 | 6169 | OWO WAT V 727 | 33.290 | 44.355 | 45.552 | 1.00 | 39.94 | 8 |
| 6128 | OWO WAT V 686 | 15.848 | 75.816 | 7.403 | 1.00 | 37.86 | 8 | 6170 | OWO WAT V 728 | 50.677 | 69.314 | 25.213 | 1.00 | 38.89 | 8 |
| 6129 | OWO WAT V 687 | 25.036 | 96.149 | 30.003 | 1.00 | 38.02 | 8 | 6171 | OWO WAT V 729 | 35.441 | 42.395 | 37.048 | 1.00 | 39.29 | 8 |
| 6130 | OWO WAT V 688 | 44.120 | 49.147 | 54.661 | 1.00 | 39.21 | 8 | 6172 | OWO WAT V 730 | 8.363 | 53.922 | 35.516 | 1.00 | 38.32 | 8 |
| 6131 | OWO WAT V 689 | 31.793 | 51.208 | 10.937 | 1.00 | 39.53 | 8 | 6173 | OWO WAT V 731 | -1.713 | 91.588 | 39.071 | 1.00 | 40.09 | 8 |
| 6132 | OWO WAT V 690 | 9.476 | 96.492 | 43.783 | 1.00 | 37.31 | 8 | 6174 | OWO WAT V 732 | 22.068 | 82.950 | 49.452 | 1.00 | 38.86 | 8 |
| 6133 | OWO WAT V 691 | 8.821 | 88.129 | 44.638 | 1.00 | 39.95 | 8 | 6175 | OWO WAT V 733 | -1.449 | 89.011 | 21.652 | 1.00 | 39.99 | 8 |
| 6134 | OWO WAT V 692 | 8.003 | 80.636 | 43.644 | 1.00 | 37.70 | 8 | 6176 | OWO WAT V 734 | 37.354 | 59.035 | 5.289 | 1.00 | 40.90 | 8 |
| 6135 | OWO WAT V 693 | 14.834 | 83.314 | 13.883 | 1.00 | 39.80 | 8 | 6177 | OWO WAT V 735 | 20.992 | 87.687 | 45.698 | 1.00 | 40.19 | 8 |
| 6136 | OWO WAT V 694 | 21.370 | 44.389 | 41.255 | 1.00 | 39.75 | 8 | 6178 | OWO WAT V 736 | 46.650 | 76.726 | 54.492 | 1.00 | 40.47 | 8 |
| 6137 | OWO WAT V 695 | 25.208 | 85.122 | 7.995 | 1.00 | 38.90 | 8 | 6179 | OWO WAT V 737 | 7.370 | 47.777 | 49.173 | 1.00 | 41.37 | 8 |
| 6138 | OWO WAT V 696 | 34.431 | 64.498 | 5.882 | 1.00 | 37.43 | 8 | 6180 | OWO WAT V 738 | 14.279 | 71.404 | 55.742 | 1.00 | 39.06 | 8 |
| 6139 | OWO WAT V 697 | 46.857 | 48.623 | 44.260 | 1.00 | 38.67 | 8 | 6181 | OWO WAT V 739 | 13.276 | 62.067 | 63.468 | 1.00 | 38.95 | 8 |
| 6140 | OWO WAT V 698 | 48.394 | 49.074 | 31.806 | 1.00 | 38.40 | 8 | 6182 | OWO WAT V 740 | 47.469 | 55.262 | 33.788 | 1.00 | 41.14 | 8 |
| 6141 | OWO WAT V 699 | 6.330 | 71.875 | 18.323 | 1.00 | 39.24 | 8 | 6183 | OWO WAT V 741 | 35.182 | 72.963 | 73.409 | 1.00 | 38.69 | 8 |
| 6142 | OWO WAT V 700 | 3.567 | 68.493 | 56.513 | 1.00 | 39.03 | 8 | 6184 | OWO WAT V 742 | 28.993 | 42.749 | 41.796 | 1.00 | 40.22 | 8 |
| 6143 | OWO WAT V 701 | 19.531 | 67.580 | 61.273 | 1.00 | 38.68 | 8 | 6185 | OWO WAT V 743 | 12.430 | 51.804 | 37.400 | 1.00 | 39.68 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 6186 | OWO WAT V 744 | 5.325 | 85.408 | 18.950 | 1.00 | 41.26 | 8 | 6228 | OWO WAT V 786 | 19.476 | 44.845 | 23.558 | 1.00 | 42.02 | 8 |
| 6187 | OWO WAT V 745 | 41.721 | 66.169 | 73.677 | 1.00 | 39.43 | 8 | 6229 | OWO WAT V 787 | 21.294 | 88.109 | 18.755 | 1.00 | 42.02 | 8 |
| 6188 | OWO WAT V 746 | 16.983 | 83.519 | 10.040 | 1.00 | 40.83 | 8 | 6230 | OWO WAT V 788 | 46.461 | 57.071 | 56.124 | 1.00 | 41.88 | 8 |
| 6189 | OWO WAT V 747 | -3.245 | 67.552 | 51.568 | 1.00 | 41.14 | 8 | 6231 | OWO WAT V 789 | 52.975 | 62.124 | 50.393 | 1.00 | 41.59 | 8 |
| 6190 | OWO WAT V 748 | 18.547 | 72.699 | 54.390 | 1.00 | 40.80 | 8 | 6232 | OWO WAT V 790 | 8.480 | 108.235 | 24.221 | 1.00 | 42.16 | 8 |
| 6191 | OWO WAT V 749 | 50.952 | 65.503 | 10.665 | 1.00 | 39.71 | 8 | 6233 | OWO WAT V 791 | 18.517 | 78.200 | 51.474 | 1.00 | 42.31 | 8 |
| 6192 | OWO WAT V 750 | 6.873 | 59.618 | 31.097 | 1.00 | 40.61 | 8 | 6234 | OWO WAT V 792 | -5.150 | 51.726 | 49.471 | 1.00 | 40.85 | 8 |
| 6193 | OWO WAT V 751 | 44.643 | 72.249 | 41.540 | 1.00 | 40.21 | 8 | 6235 | OWO WAT V 793 | 36.849 | 55.447 | 72.633 | 1.00 | 42.13 | 8 |
| 6194 | OWO WAT V 752 | 10.333 | 59.620 | 21.158 | 1.00 | 40.03 | 8 | 6236 | OWO WAT V 794 | 37.563 | 79.694 | 42.494 | 1.00 | 41.67 | 8 |
| 6195 | OWO WAT V 753 | 25.342 | 99.843 | 20.985 | 1.00 | 40.88 | 8 | 6237 | OWO WAT V 795 | 18.818 | 84.285 | 16.222 | 1.00 | 43.03 | 8 |
| 6196 | OWO WAT V 754 | 13.886 | 67.341 | 51.913 | 1.00 | 41.40 | 8 | 6238 | OWO WAT V 796 | 36.451 | 82.759 | 13.933 | 1.00 | 41.71 | 8 |
| 6197 | OWO WAT V 755 | 20.669 | 50.466 | 56.076 | 1.00 | 40.93 | 8 | 6239 | OWO WAT V 797 | 22.906 | 51.457 | 67.808 | 1.00 | 41.33 | 8 |
| 6198 | OWO WAT V 756 | 16.062 | 51.352 | 42.439 | 0.00 | 41.08 | 8 | 6240 | OWO WAT V 798 | 1.528 | 102.171 | 36.053 | 1.00 | 41.41 | 8 |
| 6199 | OWO WAT V 757 | -2.323 | 91.095 | 34.519 | 1.00 | 40.59 | 8 | 6241 | OWO WAT V 799 | 36.684 | 45.294 | 51.188 | 1.00 | 42.88 | 8 |
| 6200 | OWO WAT V 758 | 3.987 | 63.229 | 29.353 | 1.00 | 41.53 | 8 | 6242 | OWO WAT V 800 | 14.017 | 67.414 | 9.706 | 1.00 | 41.87 | 8 |
| 6201 | OWO WAT V 759 | 20.694 | 99.900 | 18.786 | 1.00 | 39.84 | 8 | 6243 | OWO WAT V 801 | 47.832 | 66.788 | 18.650 | 1.00 | 43.94 | 8 |
| 6202 | OWO WAT V 760 | 21.098 | 72.115 | 58.710 | 1.00 | 40.04 | 8 | 6244 | OWO WAT V 802 | 34.436 | 88.324 | 36.102 | 1.00 | 43.03 | 8 |
| 6203 | OWO WAT V 761 | 39.451 | 41.349 | 13.513 | 1.00 | 40.57 | 8 | 6245 | OWO WAT V 803 | 24.260 | 67.815 | 69.741 | 1.00 | 42.57 | 8 |
| 6204 | OWO WAT V 762 | 3.185 | 80.792 | 42.000 | 1.00 | 41.27 | 8 | 6246 | OWO WAT V 804 | 13.129 | 74.685 | 52.293 | 1.00 | 42.14 | 8 |
| 6205 | OWO WAT V 763 | 15.866 | 68.494 | 52.407 | 1.00 | 40.90 | 8 | 6247 | OWO WAT V 805 | 16.572 | 61.433 | 12.722 | 1.00 | 41.61 | 8 |
| 6206 | OWO WAT V 764 | 42.027 | 79.686 | 47.257 | 1.00 | 40.14 | 8 | 6248 | OWO WAT V 806 | 46.827 | 51.429 | 47.524 | 1.00 | 42.73 | 8 |
| 6207 | OWO WAT V 765 | 41.063 | 55.022 | 68.081 | 1.00 | 42.98 | 8 | 6249 | OWO WAT V 807 | 26.546 | 48.730 | 71.404 | 1.00 | 42.47 | 8 |
| 6208 | OWO WAT V 766 | 15.728 | 85.261 | 16.175 | 1.00 | 42.08 | 8 | 6250 | OWO WAT V 808 | 33.308 | 76.572 | 61.813 | 1.00 | 42.82 | 8 |
| 6209 | OWO WAT V 767 | -8.665 | 63.541 | 41.234 | 1.00 | 40.98 | 8 | 6251 | OWO WAT V 809 | 16.314 | 98.564 | 17.363 | 1.00 | 42.43 | 8 |
| 6210 | OWO WAT V 768 | 28.828 | 85.580 | 44.440 | 1.00 | 40.75 | 8 | 6252 | OWO WAT V 810 | 47.038 | 73.620 | 61.642 | 1.00 | 43.62 | 8 |
| 6211 | OWO WAT V 769 | 46.504 | 46.346 | 43.773 | 1.00 | 40.98 | 8 | 6253 | OWO WAT V 811 | 23.301 | 74.541 | 1.386 | 1.00 | 44.52 | 8 |
| 6212 | OWO WAT V 770 | 52.964 | 61.429 | 54.373 | 1.00 | 41.49 | 8 | 6254 | OWO WAT V 812 | 23.719 | 88.481 | 37.683 | 1.00 | 40.46 | 8 |
| 6213 | OWO WAT V 771 | 25.001 | 95.005 | 39.507 | 1.00 | 41.35 | 8 | 6255 | OWO WAT V 813 | 31.440 | 60.185 | 76.751 | 1.00 | 43.11 | 8 |
| 6214 | OWO WAT V 772 | 4.818 | 62.633 | 59.449 | 1.00 | 41.54 | 8 | 6256 | OWO WAT V 814 | 16.573 | 101.550 | 19.316 | 1.00 | 43.14 | 8 |
| 6215 | OWO WAT V 773 | 18.916 | 60.160 | 66.080 | 1.00 | 41.09 | 8 | 6257 | OWO WAT V 815 | 4.201 | 55.069 | 57.571 | 1.00 | 42.80 | 8 |
| 6216 | OWO WAT V 774 | 27.033 | 88.841 | 12.019 | 1.00 | 41.39 | 8 | 6258 | OWO WAT V 816 | -5.755 | 72.609 | 47.268 | 1.00 | 41.92 | 8 |
| 6217 | OWO WAT V 775 | 13.803 | 67.385 | 57.044 | 1.00 | 41.01 | 8 | 6259 | OWO WAT V 817 | 23.802 | 106.033 | 28.040 | 1.00 | 42.13 | 8 |
| 6218 | OWO WAT V 776 | 11.356 | 101.651 | 18.715 | 1.00 | 42.40 | 8 | 6260 | OWO WAT V 818 | 28.580 | 91.427 | 35.569 | 1.00 | 44.77 | 8 |
| 6219 | OWO WAT V 777 | 50.379 | 57.839 | 57.286 | 1.00 | 38.80 | 8 | 6261 | OWO WAT V 819 | -6.927 | 74.495 | 44.783 | 1.00 | 42.39 | 8 |
| 6220 | OWO WAT V 778 | 9.739 | 81.288 | 44.991 | 1.00 | 38.14 | 8 | 6262 | OWO WAT V 820 | 42.898 | 80.745 | 21.282 | 1.00 | 42.72 | 8 |
| 6221 | OWO WAT V 779 | 26.770 | 45.470 | 44.155 | 1.00 | 39.31 | 8 | 6263 | OWO WAT V 821 | 44.594 | 48.996 | 19.414 | 1.00 | 42.65 | 8 |
| 6222 | OWO WAT V 780 | 51.219 | 61.900 | 12.424 | 1.00 | 42.17 | 8 | 6264 | OWO WAT V 822 | 22.357 | 66.608 | 68.417 | 1.00 | 43.63 | 8 |
| 6223 | OWO WAT V 781 | 44.665 | 53.194 | 62.632 | 1.00 | 40.09 | 8 | 6265 | OWO WAT V 823 | 25.576 | 50.604 | 10.991 | 1.00 | 43.85 | 8 |
| 6224 | OWO WAT V 782 | -4.332 | 57.891 | 45.992 | 1.00 | 43.38 | 8 | 6266 | OWO WAT V 824 | 47.220 | 77.741 | 25.726 | 1.00 | 44.91 | 8 |
| 6225 | OWO WAT V 783 | 54.313 | 63.995 | 27.513 | 1.00 | 40.34 | 8 | 6267 | OWO WAT V 825 | 16.600 | 55.517 | 47.156 | 1.00 | 44.33 | 8 |
| 6226 | OWO WAT V 784 | 26.835 | 56.319 | 8.446 | 1.00 | 41.42 | 8 | 6268 | OWO WAT V 826 | 1.892 | 50.074 | 39.116 | 1.00 | 42.83 | 8 |
| 6227 | OWO WAT V 785 | 53.198 | 59.584 | 25.852 | 1.00 | 42.12 | 8 | 6269 | OWO WAT V 827 | 24.440 | 89.039 | 35.388 | 1.00 | 43.51 | 8 |

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|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 6270 | OWO WAT V 828 | 21.480 | 53.418 | 43.918 | 1.00 | 43.38 | 8 | 6312 | OWO WAT V 870 | 46.779 | 45.863 | 33.183 | 1.00 | 38.06 | 8 |
| 6271 | OWO WAT V 829 | 14.604 | 82.502 | 11.170 | 1.00 | 41.84 | 8 | 6313 | OWO WAT V 871 | 28.449 | 47.238 | 49.410 | 1.00 | 44.98 | 8 |
| 6272 | OWO WAT V 830 | 14.875 | 62.765 | 14.779 | 1.00 | 42.12 | 8 | 6314 | OWO WAT V 872 | 31.691 | 90.618 | 16.034 | 1.00 | 45.59 | 8 |
| 6273 | OWO WAT V 831 | 3.701 | 80.451 | 16.127 | 1.00 | 43.54 | 8 | 6315 | OWO WAT V 873 | 45.269 | 73.271 | 25.041 | 1.00 | 46.87 | 8 |
| 6274 | OWO WAT V 832 | 48.724 | 69.957 | 34.245 | 1.00 | 43.72 | 8 | 6316 | OWO WAT V 874 | 18.096 | 50.245 | 53.261 | 1.00 | 45.09 | 8 |
| 6275 | OWO WAT V 833 | 33.297 | 59.385 | 78.143 | 1.00 | 45.08 | 8 | 6317 | OWO WAT V 875 | -5.062 | 64.679 | 39.520 | 1.00 | 44.00 | 8 |
| 6276 | OWO WAT V 834 | 17.544 | 53.593 | 51.513 | 1.00 | 46.32 | 8 | 6318 | OWO WAT V 876 | 17.006 | 54.092 | 49.423 | 1.00 | 46.50 | 8 |
| 6277 | OWO WAT V 835 | 12.009 | 85.638 | 47.505 | 1.00 | 44.72 | 8 | 6319 | OWO WAT V 877 | 39.580 | 64.107 | 77.580 | 1.00 | 45.16 | 8 |
| 6278 | OWO WAT V 836 | 12.936 | 54.854 | 19.146 | 1.00 | 42.89 | 8 | 6320 | OWO WAT V 878 | 16.405 | 56.330 | 66.595 | 1.00 | 44.67 | 8 |
| 6279 | OWO WAT V 837 | 24.005 | 43.446 | 16.058 | 1.00 | 42.88 | 8 | 6321 | OWO WAT V 879 | 28.253 | 74.829 | 0.308 | 1.00 | 44.14 | 8 |
| 6280 | OWO WAT V 838 | 2.563 | 57.015 | 61.406 | 1.00 | 42.80 | 8 | 6322 | OWO WAT V 880 | 26.165 | 96.027 | 33.730 | 1.00 | 45.73 | 8 |
| 6281 | OWO WAT V 839 | 17.292 | 81.361 | 47.327 | 1.00 | 43.05 | 8 | 6323 | OWO WAT V 881 | 25.024 | 94.673 | 31.684 | 1.00 | 45.30 | 8 |
| 6282 | OWO WAT V 840 | 26.973 | 97.353 | 24.292 | 1.00 | 42.44 | 8 | 6324 | OWO WAT V 882 | 6.382 | 101.590 | 23.078 | 1.00 | 45.88 | 8 |
| 6283 | OWO WAT V 841 | 24.520 | 83.741 | 45.252 | 1.00 | 44.48 | 8 | 6325 | OWO WAT V 883 | 20.784 | 106.032 | 25.469 | 1.00 | 44.92 | 8 |
| 6284 | OWO WAT V 842 | 40.943 | 89.452 | 22.148 | 1.00 | 43.11 | 8 | 6326 | OWO WAT V 884 | 15.678 | 70.001 | 59.741 | 1.00 | 47.72 | 8 |
| 6285 | OWO WAT V 843 | 17.748 | 68.046 | 54.218 | 1.00 | 43.50 | 8 | 6327 | OWO WAT V 885 | 43.426 | 78.175 | 61.043 | 1.00 | 46.23 | 8 |
| 6286 | OWO WAT V 844 | 53.072 | 63.513 | 23.413 | 1.00 | 44.03 | 8 | 6328 | OWO WAT V 886 | 10.651 | 50.358 | 43.666 | 1.00 | 45.79 | 8 |
| 6287 | OWO WAT V 845 | -1.018 | 97.468 | 34.805 | 1.00 | 44.47 | 8 | 6329 | OWO WAT V 887 | 0.918 | 49.811 | 54.685 | 1.00 | 45.38 | 8 |
| 6288 | OWO WAT V 846 | 14.885 | 69.989 | 10.290 | 1.00 | 44.92 | 8 | 6330 | OWO WAT V 888 | 24.371 | 106.460 | 30.607 | 1.00 | 46.20 | 8 |
| 6289 | OWO WAT V 847 | 15.800 | 50.802 | 20.677 | 1.00 | 46.01 | 8 | 6331 | OWO WAT V 889 | 7.425 | 93.590 | 16.782 | 1.00 | 45.79 | 8 |
| 6290 | OWO WAT V 848 | 25.982 | 102.118 | 29.899 | 1.00 | 44.94 | 8 | 6332 | OWO WAT V 890 | 20.314 | 66.093 | 66.469 | 1.00 | 48.35 | 8 |
| 6291 | OWO WAT V 849 | 0.247 | 52.205 | 55.531 | 1.00 | 45.62 | 8 | 6333 | OWO WAT V 891 | 12.244 | 93.829 | 44.935 | 1.00 | 47.03 | 8 |
| 6292 | OWO WAT V 850 | 18.884 | 61.154 | 6.132 | 1.00 | 44.78 | 8 | 6334 | OWO WAT V 892 | 2.847 | 56.085 | 32.137 | 1.00 | 48.09 | 8 |
| 6293 | OWO WAT V 851 | 11.959 | 71.909 | 12.344 | 1.00 | 44.89 | 8 | 6335 | OWO WAT V 893 | 15.592 | 72.473 | 53.588 | 1.00 | 46.24 | 8 |
| 6294 | OWO WAT V 852 | -1.246 | 74.512 | 28.721 | 1.00 | 43.38 | 8 | 6336 | OWO WAT V 894 | 45.552 | 49.673 | 29.081 | 1.00 | 46.73 | 8 |
| 6295 | OWO WAT V 853 | 39.883 | 48.418 | 12.157 | 1.00 | 44.97 | 8 | 6337 | OWO WAT V 895 | 48.867 | 72.566 | 56.249 | 1.00 | 45.76 | 8 |
| 6296 | OWO WAT V 854 | 25.484 | 65.082 | 75.271 | 1.00 | 40.98 | 8 | 6338 | OWO WAT V 896 | 51.123 | 56.932 | 37.786 | 1.00 | 40.59 | 8 |
| 6297 | OWO WAT V 855 | 31.943 | 70.931 | 74.851 | 1.00 | 43.51 | 8 | 6339 | OWO WAT V 897 | 30.394 | 49.733 | 9.142 | 1.00 | 48.10 | 8 |
| 6298 | OWO WAT V 856 | 35.277 | 49.445 | 9.697 | 1.00 | 45.37 | 8 | 6340 | OWO WAT V 898 | 27.101 | 98.920 | 22.257 | 1.00 | 46.90 | 8 |
| 6299 | OWO WAT V 857 | 51.902 | 64.035 | 51.472 | 1.00 | 44.46 | 8 | 6341 | OWO WAT V 899 | 14.712 | 51.617 | 24.308 | 1.00 | 47.17 | 8 |
| 6300 | OWO WAT V 858 | 5.381 | 94.650 | 19.292 | 1.00 | 45.20 | 8 | 6342 | OWO WAT V 900 | 46.781 | 50.533 | 27.214 | 1.00 | 47.00 | 8 |
| 6301 | OWO WAT V 859 | 14.161 | 52.807 | 19.941 | 1.00 | 44.99 | 8 | 6343 | OWO WAT W 1 | -6.114 | 65.250 | 32.669 | 1.00 | 47.96 | 8 |
| 6302 | OWO WAT V 860 | 0.976 | 49.582 | 46.683 | 1.00 | 45.54 | 8 | 6344 | OWO WAT W 2 | 47.645 | 71.480 | 60.598 | 1.00 | 45.49 | 8 |
| 6303 | OWO WAT V 861 | 11.378 | 56.649 | 26.955 | 1.00 | 46.98 | 8 | 6345 | OWO WAT W 3 | 48.802 | 54.151 | 54.398 | 1.00 | 46.37 | 8 |
| 6304 | OWO WAT V 862 | 23.725 | 48.499 | 52.657 | 1.00 | 43.58 | 8 | 6346 | OWO WAT W 4 | 4.605 | 105.268 | 26.990 | 1.00 | 46.92 | 8 |
| 6305 | OWO WAT V 863 | 31.619 | 53.767 | 4.982 | 1.00 | 44.03 | 8 | 6347 | OWO WAT W 5 | 42.143 | 73.136 | 41.061 | 1.00 | 45.02 | 8 |
| 6306 | OWO WAT V 864 | 21.564 | 85.158 | 16.121 | 1.00 | 46.34 | 8 | 6348 | OWO WAT W 6 | 26.105 | 89.154 | 41.563 | 1.00 | 47.90 | 8 |
| 6307 | OWO WAT V 865 | 48.454 | 57.833 | 31.207 | 1.00 | 45.05 | 8 | 6349 | OWO WAT W 7 | 3.202 | 48.853 | 55.140 | 1.00 | 47.23 | 8 |
| 6308 | OWO WAT V 866 | 13.820 | 78.070 | 11.134 | 1.00 | 47.52 | 8 | 6350 | OWO WAT W 8 | -2.318 | 61.724 | 33.458 | 1.00 | 48.00 | 8 |
| 6309 | OWO WAT V 867 | 53.268 | 61.611 | 27.715 | 1.00 | 45.47 | 8 | 6351 | OWO WAT W 9 | 38.569 | 50.803 | 7.204 | 1.00 | 46.95 | 8 |
| 6310 | OWO WAT V 868 | 40.661 | 42.455 | 21.732 | 1.00 | 43.57 | 8 | 6352 | OWO WAT W 10 | 2.160 | 103.336 | 25.390 | 1.00 | 47.08 | 8 |
| 6311 | OWO WAT V 869 | 24.881 | 97.609 | 17.754 | 1.00 | 41.56 | 8 | 6353 | OWO WAT W 11 | 27.464 | 41.903 | 36.189 | 1.00 | 42.96 | 8 |

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|------|--------------|--------|---------|--------|------------|---|------|--------------|--------|---------|--------|------------|---|
| 6354 | OWO WAT W 12 | 49.209 | 50.152 | 22.583 | 1.00 48.25 | 8 | 6396 | OWO WAT W 54 | 49.464 | 48.219 | 14.354 | 1.00 55.58 | 8 |
| 6355 | OWO WAT W 13 | 10.266 | 57.487 | 62.131 | 1.00 43.39 | 8 | 6397 | OWO WAT W 55 | -2.823 | 49.394 | 48.028 | 1.00 50.11 | 8 |
| 6356 | OWO WAT W 14 | 54.127 | 66.185 | 63.244 | 1.00 49.78 | 8 | 6398 | OWO WAT W 56 | 22.263 | 105.611 | 23.242 | 1.00 50.89 | 8 |
| 6357 | OWO WAT W 15 | 19.083 | 49.330 | 63.179 | 1.00 49.30 | 8 | 6399 | OWO WAT W 57 | 16.395 | 151.479 | 56.998 | 1.00 54.48 | 8 |
| 6358 | OWO WAT W 16 | 39.385 | 74.287 | 38.793 | 1.00 46.50 | 8 | 6400 | OWO WAT W 58 | 46.461 | 51.028 | 12.082 | 1.00 51.52 | 8 |
| 6359 | OWO WAT W 17 | -1.255 | 52.062 | 41.948 | 1.00 49.09 | 8 | 6401 | OWO WAT W 59 | 35.996 | 61.651 | 5.602 | 1.00 53.96 | 8 |
| 6360 | OWO WAT W 18 | 16.630 | 69.708 | 8.569 | 1.00 48.63 | 8 | 6402 | OWO WAT W 60 | 25.277 | 46.888 | 50.958 | 1.00 53.30 | 8 |
| 6361 | OWO WAT W 19 | 29.289 | 54.314 | 9.208 | 1.00 49.09 | 8 | 6403 | OWO WAT W 61 | 15.763 | 94.604 | 17.487 | 1.00 49.77 | 8 |
| 6362 | OWO WAT W 20 | 38.590 | 83.950 | 31.916 | 1.00 48.14 | 8 | 6404 | OWO WAT W 62 | 42.937 | 61.534 | 7.934 | 1.00 47.74 | 8 |
| 6363 | OWO WAT W 21 | 47.212 | 44.923 | 37.558 | 1.00 49.07 | 8 | 6405 | OWO WAT W 63 | 24.840 | 46.516 | 44.072 | 1.00 51.69 | 8 |
| 6364 | OWO WAT W 22 | 2.016 | 104.557 | 33.998 | 1.00 50.31 | 8 | 6406 | OWO WAT W 64 | 29.111 | 92.028 | 40.197 | 1.00 48.35 | 8 |
| 6365 | OWO WAT W 23 | 5.910 | 79.410 | 15.810 | 1.00 46.74 | 8 | 6407 | OWO WAT W 65 | 4.689 | 89.221 | 19.393 | 1.00 50.44 | 8 |
| 6366 | OWO WAT W 24 | 18.824 | 46.920 | 16.693 | 1.00 44.54 | 8 | 6408 | OWO WAT W 66 | 11.456 | 93.383 | 15.046 | 1.00 58.07 | 8 |
| 6367 | OWO WAT W 25 | 21.253 | 90.457 | 18.335 | 1.00 47.12 | 8 | 6409 | OWO WAT W 67 | 15.227 | 108.500 | 35.816 | 1.00 52.43 | 8 |
| 6368 | OWO WAT W 26 | 46.674 | 72.576 | 34.746 | 1.00 48.69 | 8 | 6410 | OWO WAT W 68 | 42.860 | 74.904 | 32.815 | 1.00 52.70 | 8 |
| 6369 | OWO WAT W 27 | 17.804 | 54.470 | 14.884 | 1.00 50.05 | 8 | 6411 | OWO WAT W 69 | 48.829 | 69.006 | 23.605 | 1.00 55.19 | 8 |
| 6370 | OWO WAT W 28 | -3.319 | 64.779 | 54.655 | 1.00 49.95 | 8 | 6412 | OWO WAT W 70 | 15.485 | 68.666 | 11.962 | 1.00 52.48 | 8 |
| 6371 | OWO WAT W 29 | 20.035 | 59.810 | 69.328 | 1.00 47.36 | 8 | 6413 | OWO WAT W 71 | -5.047 | 98.836 | 30.411 | 1.00 52.33 | 8 |
| 6372 | OWO WAT W 30 | 6.598 | 98.214 | 19.529 | 1.00 50.29 | 8 | 6414 | OWO WAT W 72 | 38.899 | 69.928 | 3.024 | 1.00 53.43 | 8 |
| 6373 | OWO WAT W 31 | 29.388 | 57.634 | 5.275 | 1.00 49.23 | 8 | 6415 | OWO WAT W 73 | 47.563 | 47.253 | 16.948 | 1.00 53.16 | 8 |
| 6374 | OWO WAT W 32 | 25.881 | 83.371 | 19.453 | 1.00 49.89 | 8 | 6416 | OWO WAT W 74 | 8.621 | 51.721 | 57.810 | 1.00 51.63 | 8 |
| 6375 | OWO WAT W 33 | 46.828 | 48.534 | 13.616 | 1.00 48.17 | 8 | 6417 | OWO WAT W 75 | 52.887 | 59.020 | 49.147 | 1.00 50.28 | 8 |
| 6376 | OWO WAT W 34 | 52.912 | 62.999 | 14.852 | 1.00 46.56 | 8 | 6418 | OWO WAT W 76 | 4.037 | 61.529 | 30.846 | 1.00 54.62 | 8 |
| 6377 | OWO WAT W 35 | 2.107 | 83.103 | 18.070 | 1.00 48.10 | 8 | 6419 | OWO WAT W 77 | 4.332 | 83.232 | 16.091 | 1.00 55.82 | 8 |
| 6378 | OWO WAT W 36 | 41.486 | 67.797 | 7.736 | 1.00 50.23 | 8 | 6420 | OWO WAT W 78 | 36.037 | 53.977 | 74.978 | 1.00 55.15 | 8 |
| 6379 | OWO WAT W 37 | 9.492 | 94.962 | 15.817 | 1.00 48.00 | 8 | 6421 | OWO WAT W 79 | 51.512 | 53.978 | 47.701 | 0.00 54.18 | 8 |
| 6380 | OWO WAT W 38 | 28.348 | 95.134 | 21.001 | 1.00 48.19 | 8 | 6422 | OWO WAT W 80 | 14.797 | 91.920 | 17.273 | 1.00 51.87 | 8 |
| 6381 | OWO WAT W 39 | 32.401 | 92.434 | 25.439 | 1.00 50.58 | 8 | 6423 | OWO WAT W 81 | 19.801 | 84.369 | 8.356 | 1.00 55.63 | 8 |
| 6382 | OWO WAT W 40 | 46.035 | 46.956 | 48.050 | 1.00 50.92 | 8 | 6424 | OWO WAT W 82 | 31.496 | 46.252 | 52.107 | 1.00 55.15 | 8 |
| 6383 | OWO WAT W 41 | 34.909 | 51.572 | 71.159 | 1.00 49.38 | 8 | 6425 | OWO WAT W 83 | -1.823 | 79.829 | 19.762 | 1.00 53.76 | 8 |
| 6384 | OWO WAT W 42 | 29.114 | 76.486 | 61.672 | 1.00 49.83 | 8 | 6426 | OWO WAT W 84 | 29.256 | 92.834 | 20.731 | 1.00 53.49 | 8 |
| 6385 | OWO WAT W 43 | -3.044 | 91.942 | 40.975 | 1.00 51.92 | 8 | 6427 | OWO WAT W 85 | -1.824 | 76.279 | 32.563 | 1.00 55.76 | 8 |
| 6386 | OWO WAT W 44 | -3.395 | 74.451 | 28.328 | 1.00 46.84 | 8 | 6428 | OWO WAT W 86 | 32.061 | 46.088 | 49.588 | 1.00 55.95 | 8 |
| 6387 | OWO WAT W 45 | 20.187 | 89.421 | 44.602 | 1.00 49.88 | 8 | 6429 | OWO WAT W 87 | 41.327 | 42.439 | 33.669 | 1.00 55.86 | 8 |
| 6388 | OWO WAT W 46 | -4.080 | 54.699 | 41.545 | 1.00 50.13 | 8 | 6430 | OWO WAT W 88 | 43.153 | 80.324 | 3.532 | 1.00 52.67 | 8 |
| 6389 | OWO WAT W 47 | 38.425 | 87.733 | 31.621 | 1.00 49.47 | 8 | 6431 | OWO WAT W 89 | 47.799 | 76.801 | 61.841 | 1.00 55.93 | 8 |
| 6390 | OWO WAT W 48 | 4.305 | 62.413 | 62.323 | 1.00 49.60 | 8 | 6432 | OWO WAT W 90 | 35.708 | 85.333 | 37.348 | 1.00 54.64 | 8 |
| 6391 | OWO WAT W 49 | 6.229 | 89.367 | 44.095 | 1.00 53.06 | 8 | 6433 | OWO WAT W 91 | 52.110 | 65.452 | 56.038 | 1.00 53.77 | 8 |
| 6392 | OWO WAT W 50 | 49.747 | 66.902 | 23.155 | 0.00 51.47 | 8 | 6434 | OWO WAT W 92 | 16.996 | 79.167 | 47.458 | 1.00 56.65 | 8 |
| 6393 | OWO WAT W 51 | 40.855 | 78.417 | 26.292 | 1.00 48.79 | 8 | 6435 | OWO WAT W 93 | 27.626 | 49.502 | 11.515 | 1.00 60.46 | 8 |
| 6394 | OWO WAT W 52 | 17.489 | 50.714 | 66.895 | 1.00 52.19 | 8 | 6436 | OWO WAT W 94 | 29.317 | 47.547 | 14.906 | 1.00 61.23 | 8 |
| 6395 | OWO WAT W 53 | 34.327 | 92.622 | 27.782 | 1.00 49.40 | 8 | 6437 | OWO WAT W 95 | 51.306 | 65.455 | 30.794 | 0.00 67.31 | 8 |

| | | | | | | | | | | | | | | | |
|------|---------------|--------|---------|--------|------|-------|---|------|---------------|--------|---------|--------|------|-------|---|
| 6438 | OWO WAT W 96 | 21.436 | 52.799 | 12.475 | 1.00 | 60.39 | 8 | 6480 | OWO WAT W 138 | 38.033 | 48.935 | 8.928 | 1.00 | 56.21 | 8 |
| 6439 | OWO WAT W 97 | 24.857 | 50.122 | 68.228 | 1.00 | 61.97 | 8 | 6481 | OWO WAT W 139 | 22.720 | 48.167 | 43.406 | 1.00 | 43.05 | 8 |
| 6440 | OWO WAT W 98 | 53.436 | 60.942 | 47.809 | 1.00 | 59.88 | 8 | 6482 | OWO WAT W 140 | 16.160 | 51.440 | 42.398 | 1.00 | 42.33 | 8 |
| 6441 | OWO WAT W 99 | 26.545 | 99.863 | 28.613 | 1.00 | 66.13 | 8 | 6483 | OWO WAT W 141 | 51.286 | 65.520 | 30.747 | 0.00 | 58.93 | 8 |
| 6442 | OWO WAT W 100 | 28.187 | 94.100 | 34.809 | 1.00 | 47.55 | 8 | 6484 | OWO WAT W 142 | 22.870 | 83.783 | -0.279 | 1.00 | 39.91 | 8 |
| 6443 | OWO WAT W 101 | 46.501 | 68.477 | 9.327 | 1.00 | 62.49 | 8 | 6485 | OWO WAT W 143 | 23.492 | 85.411 | 14.742 | 1.00 | 45.55 | 8 |
| 6444 | OWO WAT W 102 | 41.335 | 80.622 | 32.546 | 1.00 | 56.46 | 8 | 6486 | OWO WAT W 144 | 30.609 | 38.135 | 34.869 | 1.00 | 53.23 | 8 |
| 6445 | OWO WAT W 103 | 49.090 | 47.019 | 29.937 | 1.00 | 51.60 | 8 | 6487 | OWO WAT W 145 | 51.546 | 53.971 | 47.725 | 0.00 | 54.90 | 8 |
| 6446 | OWO WAT W 104 | 29.677 | 70.505 | 75.480 | 1.00 | 55.52 | 8 | 6488 | OWO WAT W 146 | 37.344 | 40.493 | 33.234 | 1.00 | 46.02 | 8 |
| 6447 | OWO WAT W 105 | 10.580 | 70.552 | 56.020 | 1.00 | 45.60 | 8 | 6489 | OWO WAT W 147 | 35.805 | 47.572 | 62.190 | 1.00 | 53.24 | 8 |
| 6448 | OWO WAT W 106 | -5.437 | 61.460 | 36.195 | 1.00 | 49.58 | 8 | 6490 | OWO WAT W 148 | 32.439 | 62.293 | 76.111 | 1.00 | 52.51 | 8 |
| 6449 | OWO WAT W 107 | 41.636 | 42.378 | 28.372 | 1.00 | 47.73 | 8 | 6491 | OWO WAT W 149 | 24.077 | 90.751 | 37.673 | 1.00 | 48.00 | 8 |
| 6450 | OWO WAT W 108 | 48.134 | 51.375 | 29.584 | 1.00 | 53.67 | 8 | 6492 | OWO WAT W 150 | 20.655 | 50.869 | 68.464 | 1.00 | 51.34 | 8 |
| 6451 | OWO WAT W 109 | 20.029 | 46.534 | 41.141 | 1.00 | 45.69 | 8 | 6493 | OWO WAT W 151 | 42.359 | 76.800 | 31.368 | 1.00 | 54.68 | 8 |
| 6452 | OWO WAT W 110 | 39.076 | 61.857 | 77.827 | 1.00 | 61.24 | 8 | 6494 | OWO WAT W 152 | 40.991 | 84.869 | 28.522 | 1.00 | 51.94 | 8 |
| 6453 | OWO WAT W 111 | 40.140 | 79.602 | 28.296 | 1.00 | 58.08 | 8 | 6495 | OWO WAT W 153 | -3.448 | 59.486 | 34.298 | 1.00 | 60.14 | 8 |
| 6454 | OWO WAT W 112 | 24.479 | 41.686 | 38.003 | 1.00 | 48.71 | 8 | 6496 | OWO WAT W 154 | 24.275 | 50.044 | 65.629 | 1.00 | 48.99 | 8 |
| 6455 | OWO WAT W 113 | 18.748 | 86.522 | 18.736 | 1.00 | 54.95 | 8 | 6497 | OWO WAT W 155 | 24.898 | 47.635 | 57.042 | 1.00 | 50.00 | 8 |
| 6456 | OWO WAT W 114 | 26.670 | 86.155 | 43.878 | 1.00 | 45.83 | 8 | 6498 | OWO WAT W 156 | 46.911 | 73.376 | 32.086 | 1.00 | 65.97 | 8 |
| 6457 | OWO WAT W 115 | 34.014 | 44.101 | 58.947 | 1.00 | 55.80 | 8 | 6499 | OWO WAT W 157 | 12.448 | 63.643 | 14.806 | 1.00 | 50.68 | 8 |
| 6458 | OWO WAT W 116 | 44.085 | 44.358 | 32.579 | 1.00 | 66.42 | 8 | 6500 | OWO WAT W 158 | 17.367 | 83.516 | 7.750 | 1.00 | 59.03 | 8 |
| 6459 | OWO WAT W 117 | 2.549 | 102.526 | 41.260 | 1.00 | 56.37 | 8 | 6501 | OWO WAT W 159 | 38.537 | 87.429 | 19.244 | 1.00 | 48.05 | 8 |
| 6460 | OWO WAT W 118 | 10.042 | 59.115 | 64.251 | 1.00 | 53.53 | 8 | 6502 | OWO WAT W 160 | 49.397 | 68.482 | 30.753 | 0.00 | 47.12 | 8 |
| 6461 | OWO WAT W 119 | 52.498 | 59.271 | 37.676 | 1.00 | 46.44 | 8 | 6503 | OWO WAT W 161 | 52.562 | 62.737 | 30.460 | 0.00 | 55.04 | 8 |
| 6462 | OWO WAT W 120 | 49.412 | 68.479 | 30.738 | 0.00 | 48.32 | 8 | 6504 | OWO WAT W 162 | 17.100 | 92.730 | 17.506 | 1.00 | 48.89 | 8 |
| 6463 | OWO WAT W 121 | 39.604 | 81.174 | 29.899 | 1.00 | 40.72 | 8 | 6505 | OWO WAT W 163 | 54.143 | 65.666 | 53.272 | 1.00 | 49.78 | 8 |
| 6464 | OWO WAT W 122 | 52.578 | 62.726 | 30.463 | 0.00 | 55.27 | 8 | 6506 | OWO WAT W 164 | 35.140 | 89.217 | 21.335 | 0.00 | 49.55 | 8 |
| 6465 | OWO WAT W 123 | 32.284 | 38.992 | 32.423 | 1.00 | 44.19 | 8 | 6507 | OWO WAT W 165 | 40.864 | 85.144 | 25.201 | 1.00 | 51.96 | 8 |
| 6466 | OWO WAT W 124 | 54.342 | 58.298 | 13.900 | 1.00 | 48.84 | 8 | 6508 | OWO WAT W 166 | 0.129 | 71.062 | 53.859 | 1.00 | 50.46 | 8 |
| 6467 | OWO WAT W 125 | 53.831 | 60.018 | 17.609 | 1.00 | 53.12 | 8 | 6509 | OWO WAT W 167 | 19.749 | 95.732 | 16.395 | 1.00 | 54.02 | 8 |
| 6468 | OWO WAT W 126 | 37.548 | 48.910 | 67.790 | 1.00 | 63.29 | 8 | 6510 | OWO WAT W 168 | 45.089 | 55.696 | 66.763 | 1.00 | 48.69 | 8 |
| 6469 | OWO WAT W 127 | 16.364 | 67.201 | 64.210 | 1.00 | 54.77 | 8 | 6511 | OWO WAT W 169 | 29.920 | 93.952 | 27.969 | 1.00 | 57.82 | 8 |
| 6470 | OWO WAT W 128 | 35.507 | 88.726 | 18.930 | 1.00 | 44.18 | 8 | 6512 | OWO WAT W 170 | -1.140 | 103.281 | 29.038 | 1.00 | 59.68 | 8 |
| 6471 | OWO WAT W 129 | 49.585 | 56.011 | 59.240 | 1.00 | 44.54 | 8 | 6513 | OWO WAT W 171 | 0.493 | 67.332 | 27.261 | 1.00 | 46.75 | 8 |
| 6472 | OWO WAT W 130 | 13.470 | 54.095 | 28.765 | 1.00 | 39.17 | 8 | 6514 | OWO WAT W 172 | 11.663 | 49.273 | 52.961 | 1.00 | 47.65 | 8 |
| 6473 | OWO WAT W 131 | 11.141 | 90.680 | 16.198 | 1.00 | 49.46 | 8 | 6515 | OWO WAT W 173 | 19.395 | 43.670 | 27.536 | 0.00 | 52.64 | 8 |
| 6474 | OWO WAT W 132 | -9.184 | 65.150 | 46.616 | 1.00 | 52.99 | 8 | 6516 | OWO WAT W 174 | 12.558 | 73.429 | 10.221 | 1.00 | 52.09 | 8 |
| 6475 | OWO WAT W 133 | 44.910 | 67.182 | 7.757 | 1.00 | 52.67 | 8 | 6517 | OWO WAT W 175 | 47.725 | 72.168 | 25.475 | 1.00 | 55.03 | 8 |
| 6476 | OWO WAT W 134 | 38.968 | 68.370 | 71.252 | 1.00 | 37.18 | 8 | 6518 | OWO WAT W 176 | 37.354 | 46.525 | 53.992 | 1.00 | 62.86 | 8 |
| 6477 | OWO WAT W 135 | 9.962 | 106.661 | 35.598 | 1.00 | 48.81 | 8 | 6519 | OWO WAT W 177 | 6.566 | 77.689 | 48.060 | 1.00 | 54.04 | 8 |
| 6478 | OWO WAT W 136 | -0.018 | 83.329 | 37.562 | 1.00 | 49.93 | 8 | 6520 | OWO WAT W 178 | 27.239 | 80.756 | 54.362 | 1.00 | 54.49 | 8 |
| 6479 | OWO WAT W 137 | 6.077 | 95.625 | 42.890 | 1.00 | 41.31 | 8 | 6521 | OWO WAT W 179 | 29.136 | 79.115 | 59.854 | 1.00 | 51.47 | 8 |

| | | | | | | | | | | |
|------|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| 6522 | OWO | WAT | W | 180 | 51.301 | 65.512 | 30.778 | 1.00 | 58.87 | 8 |
| 6523 | OWO | WAT | W | 181 | 49.729 | 67.077 | 23.232 | 1.00 | 50.64 | 8 |
| 6524 | OWO | WAT | W | 182 | 15.428 | 63.127 | 65.725 | 1.00 | 53.21 | 8 |
| 6525 | OWO | WAT | W | 183 | 28.316 | 47.473 | 59.001 | 1.00 | 52.58 | 8 |
| 6526 | OWO | WAT | W | 184 | 11.167 | 50.777 | 21.789 | 1.00 | 55.21 | 8 |
| 6527 | OWO | WAT | W | 185 | 39.667 | 45.779 | 11.484 | 1.00 | 50.46 | 8 |
| 6528 | OWO | WAT | W | 186 | 9.302 | 78.481 | 48.408 | 1.00 | 50.14 | 8 |
| 6529 | OWO | WAT | W | 187 | -2.511 | 95.777 | 25.082 | 1.00 | 50.26 | 8 |
| 6530 | OWO | WAT | W | 188 | 49.525 | 52.221 | 41.616 | 1.00 | 53.78 | 8 |
| 6531 | OWO | WAT | W | 189 | 33.219 | 90.787 | 32.195 | 1.00 | 53.22 | 8 |
| 6532 | OWO | WAT | W | 190 | 18.629 | 63.971 | 67.355 | 1.00 | 54.97 | 8 |
| 6533 | OWO | WAT | W | 191 | 6.996 | 55.402 | 34.790 | 1.00 | 49.49 | 8 |
| 6534 | OWO | WAT | W | 192 | 50.269 | 70.807 | 60.070 | 1.00 | 54.80 | 8 |
| 6535 | OWO | WAT | W | 193 | -3.948 | 89.479 | 31.518 | 0.00 | 54.80 | 8 |
| 6536 | OWO | WAT | W | 194 | 4.036 | 51.795 | 57.529 | 1.00 | 56.49 | 8 |
| 6537 | OWO | WAT | W | 195 | 15.790 | 48.084 | 23.036 | 1.00 | 52.39 | 8 |
| 6538 | OWO | WAT | W | 196 | 22.577 | 105.708 | 45.361 | 1.00 | 51.14 | 8 |
| 6539 | OWO | WAT | W | 197 | 7.453 | 103.921 | 23.508 | 1.00 | 50.15 | 8 |
| 6540 | OWO | WAT | W | 198 | 37.899 | 80.588 | 45.384 | 1.00 | 52.20 | 8 |
| 6541 | OWO | WAT | W | 199 | 19.774 | 74.879 | 53.890 | 1.00 | 55.07 | 8 |
| 6542 | OWO | WAT | W | 200 | 50.055 | 68.873 | 30.956 | 1.00 | 30.00 | 8 |
| 6543 | OWO | WAT | W | 201 | 53.330 | 63.201 | 30.956 | 1.00 | 37.00 | 8 |
| 6544 | OWO | WAT | W | 202 | 35.086 | 89.130 | 21.284 | 1.00 | 49.00 | 8 |
| 6545 | OWO | WAT | W | 203 | 2.339 | 51.858 | 35.796 | 1.00 | 50.00 | 8 |
| 6546 | OWO | WAT | W | 204 | 19.180 | 43.755 | 27.572 | 1.00 | 50.00 | 8 |
| 6547 | OWO | WAT | W | 205 | 51.693 | 55.504 | 46.921 | 1.00 | 51.00 | 8 |
| 6548 | OWO | WAT | W | 206 | 31.811 | 80.217 | 54.661 | 1.00 | 51.00 | 8 |
| 6549 | OWO | WAT | W | 207 | 11.695 | 77.786 | 12.093 | 1.00 | 51.00 | 8 |
| 6550 | OWO | WAT | W | 208 | 29.940 | 46.996 | 53.693 | 1.00 | 52.00 | 8 |
| 6551 | OWO | WAT | W | 209 | 7.251 | 102.500 | 40.633 | 1.00 | 52.00 | 8 |
| 6552 | OWO | WAT | W | 210 | 23.858 | 91.561 | 17.414 | 1.00 | 52.00 | 8 |
| 6553 | OWO | WAT | W | 211 | 6.783 | 49.832 | 40.633 | 1.00 | 52.00 | 8 |
| 6554 | OWO | WAT | W | 212 | 44.910 | 47.806 | 22.735 | 1.00 | 52.00 | 8 |
| 6555 | OWO | WAT | W | 213 | 36.255 | 46.591 | 10.158 | 1.00 | 52.00 | 8 |
| 6556 | OWO | WAT | W | 214 | 27.601 | 61.581 | 77.880 | 1.00 | 52.00 | 8 |
| 6557 | OWO | WAT | W | 215 | 27.133 | 98.043 | 33.861 | 1.00 | 53.00 | 8 |
| 6558 | OWO | WAT | W | 216 | 18.479 | 55.504 | 45.470 | 1.00 | 53.00 | 8 |
| 6559 | OWO | WAT | W | 217 | 9.122 | 47.401 | 46.438 | 1.00 | 53.00 | 8 |
| 6560 | OWO | WAT | W | 218 | 9.590 | 66.037 | 16.447 | 1.00 | 53.00 | 8 |
| 6561 | OWO | WAT | W | 219 | 13.333 | 91.966 | 46.438 | 1.00 | 53.00 | 8 |

CLAIMS:

1. A method of producing a variant of a parent maltogenic alpha-amylase, said method comprising
 - a) modeling the parent alpha-amylase on the three-dimensional structure of SEQ ID NO: 1 depicted in the Appendix to produce a three-dimensional structure of the parent alpha-amylase;
 - b) identifying in the three-dimensional structure obtained in step (a) at least one structural part of the parent wherein an alteration in said structural part is predicted to result in said altered property;
 - c) modifying the sequence of a nucleic acid encoding the parent alpha-amylase to produce a nucleic acid encoding a deletion, insertion, or substitution of one or more amino acids at a position corresponding to said structural part; and
 - d) expressing the modified nucleic acid in a host cell to produce the variant alpha-amylase,wherein the variant has alpha-amylase enzymatic activity and has at least one altered property relative to the parent.
2. The method of claim 1, wherein the altered property is pH dependent activity, thermostability, substrate cleavage pattern, specific activity of cleavage, transglycosylation, ability to reduce retrogradation of starch, ability to reduce staling of bread, substrate specificity, substrate binding or calcium binding.
3. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:
 - a) identifying an amino acid residue which is within 15 Å (in particular 10 Å) from an active site residue of the parent amylase in the three-dimensional structure of said parent, and which is involved in electrostatic or hydrophobic interactions with an active site residue;
 - b) substituting said amino acid residue with another amino acid residue which changes the electrostatic and/or hydrophobic surroundings of an active site residue, and which can be accommodated in the structure;
 - c) optionally repeating steps a) and b) recursively;
 - d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),

- e) preparing the variant resulting from steps a) - d);
- f) testing the pH dependent activity of said variant; and
- g) optionally repeating steps a) - f) recursively; and
- h) selecting a variant having an altered pH dependent activity as compared
5 to the parent amylase.

4. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- a) identifying an internal cavity or crevice in the three-dimensional structure of said parent;
- 10 b) substituting an amino acid residue in the neighborhood of the cavity or crevice with another amino acid residue which increases the hydrophobic interaction and/or fills out or reduces the size of the cavity or crevice;
- c) optionally repeating steps a) and b) recursively;
- d) optionally, making alterations each of which is an insertion, a deletion or a
15 substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the thermostability of said variant; and
- g) optionally repeating steps a) - f) recursively; and
- h) selecting a variant having increased thermostability as compared to the
20 parent amylase.

5. The method of claim 4, wherein the substitution of the amino acid residue results in increasing the hydrophobic interaction, substitution with proline, substitution of histidine with another amino acid, stabilization of calcium binding, introduction of an interdomain disulfide bond, removal of a deamidation site, altering a hydrogen
25 bond contact, filling in an internal structural cavity with an amino acid with a bulkier side group, introduction of interdomain interactions, altering charge distribution, helix capping, or introduction of a salt bridge.

6. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- 30 a) identifying an amino acid residue within 10 Å from a calcium binding site in the three dimensional structure of the amylase;
- b) substituting the amino acid residue with another amino acid residue so as to improve the interaction with the calcium ion;
- c) optionally repeating steps a) and b) recursively;

- d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the thermostability of said variant; and
- 5 g) optionally repeating steps a) - f) recursively; and
- h) selecting a variant having increased thermostability as compared to the parent amylase.

7. A method of constructing a variant of a parent maltogenic alpha-amylase, which method comprises:

- 10 a) identifying the substrate binding area in a model of the three-dimensional structure of the parent amylase;
- b) modifying the substrate binding area by an amino acid substitution, deletion or insertion;
- c) optionally repeating step b) recursively;
- 15 d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b),
- e) preparing the variant resulting from steps a) - d);
- f) testing the substrate-cleavage pattern of the variant.
- g) optionally repeating steps a) - f) recursively; and
- 20 h) selecting a variant having an altered substrate-cleavage pattern as compared to the parent amylase.

8. A method for producing a maltogenic alpha-amylase variant, comprising:

- a) constructing the variant by the method of any of claims 2-7;
- b) transforming a microorganism with a DNA sequence encoding the variant;
- 25 c) cultivating the transformed microorganism under conditions which are conducive for producing the variant, and
- d) optionally, recovering the variant from the resulting culture broth.

9. A polypeptide which:

- a) has maltogenic alpha-amylase activity;
- 30 b) has at least 70 % identity to SEQ ID NO: 1;
- c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to D127, V129, F188, A229, Y258, V281, F284, T288, N327, M330, G370, N371, and/or D372; and
- d) has altered pH dependent activity as compared to the polypeptide of SEQ
- 35 ID NO: 1.

10. The polypeptide of claim 9, wherein the modification comprises a substitution corresponding to D127N/L, V129S/T/G/V, F188E/K/H, A229S/T/G/V, Y258E/D/K/R/F/N, V281L/T, F284K/H/D/E/Y, T288E/K/R, N327D, M330L/F/I/D/E/K, G370N, N371D/E/G/K, and/or D372N/V.

5 11. A polypeptide which:

- a) has maltogenic alpha-amylase activity;
- b) has at least 70 % identity to SEQ ID NO: 1; and
- c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to Q13, I16, D17, N26, N28, P29, A30, S32, Y33, G34, L35, K40, M45, P73, V74, D76, N77, D79, N86, R95, N99, I100, H103, Q119, N120, N131, S141, T142, A148, N152, A163, H169, N171, G172, I174, N176, N187, F188, A192, Q201, N203, H220, N234, G236, Q247, K249, D261, N266, L268, R272, N275, N276, V279, N280, V281, D285, N287, F297, Q299, N305, K316, N320, L321, N327, A341, N342, A348, Q365, N371, N375, M378, G397, A381, F389, N401, A403, K425, N436, S442, N454, N468, N474, S479, A483, A486, V487, S493, T494, S495, A496, S497, A498, Q500, N507, I510, N513, K520, Q526, A555, A564, S573, N575, Q581, S583, F586, K589, N595, G618, N621, Q624, A629, F636, K645, N664 and/or T681; and
- d) has improved stability compared to the polypeptide of SEQ ID NO: 1.

20 12. The polypeptide of claim 11, wherein the modification comprises at a position corresponding to K40, V74, H103, S141, T142, F188, H220, N234, K249, D261, L268, V279, N342, H344, G397, A403, K425, S442, S479, S493, T494, S495, A496, S497, A498, Q500, K520, A555 and/or N595; preferably a substitution corresponding to K40R, V74P, H103Y/V/I/L/F/Y, S141P, T142A, F188I/L, H220Y/L/M, N234P, K249P, D261G, L268P, V279P, N342P, H344E/Q/N/D/Y, G397P, A403P, K425E, S442P, S479P, S493P, T494P, S495P, A496P, S497P, A498P, Q500P, K520R, A555P and/or N595I.

13. The polypeptide of claim 11 or 12, wherein the modification comprises at a position corresponding to D17, N28, P29, A30, S32, Y33, G34, R95, H103, N131, H169, I174 and/or Q201 such as to improve calcium coordination, preferably a substitution corresponding to D17Q/E, A30D/M/L/A/V/I/E/Q, S32D/E/N/Q, R95M/L/A/V/I/E/Q, H103Y/N/Q/D/E, N131D, H169N/D/E/Q, I174E/Q, Q201E.

14. The polypeptide of any of claims 11-13, wherein the modification comprises a substitution at a position corresponding to Q13, N26, N77, N86, N99, Q119, N120,

- N131, N152, N171, N176, N187, Q201, N203, N234, Q247, N266, N275, N276, N280, N287, Q299, N320, N327, N342, Q365, N371, N375, N401, N436, N454, N468, N474, Q500, N507, N513, Q526, N575, Q581, N621, Q624 and/or N664 such as to remove a deamidation site, preferably a substitution corresponding to
- 5 Q13S/T/A/V/L/I/F/M, N26S/T/A/V/L/I, N77S/T/A/V/L/I, N86S/T/A/V/L/I, N99T/S/V/L, Q119T/S, N120S/T/A/V/L/I, N131S/T/A/V/L/I, N152T/S/V/L, N171Y/D/S/T, N176S/T/A/V/L/I, N187S/T/A/V/L/I, Q201S/T/A/V/L/I/F/M, N203D/S/T/A/V/L/I, N234S/T/A/V/L/I, Q247S/T/A/V/L/I/F/M, N266S/T/A/V/L/I, N275S/T/A/V/L/I, N276S/T/A/V/L/I, N280S/T/A/V/L/I, N287S/T/A/V/L/I, Q299L/T/S, N320S/T/A/V/L/I,
- 10 N327S/T/A/V/L/I, N342S/T/A/V/L/I, Q365S/T/A/V/L/I, N371S/T/A/V/L/I, N375S/T/A/V/L/I, N401S/T/A/V/L/I, N436S/T/A/V/L/I, N454D/S/T/A/V/L/I, N468D/S/T/A/V/L/I, N474D/S/T/A/V/L/I, Q500S/T/A/V/L/I/F/M, N507S/T/A/V/L/I, N513S/T/A/V/L/I, Q526 D/S/T/A/V/L/I, N575S/T/A/V/L/I, Q581S/T/A/V/L/I/F/M, N621S/T/A/V/L/I Q624S/T/A/V/L/I/F/M and/or N664D/S/T/A/V/L/I.
- 15 15. The polypeptide of any of claims 11-14, wherein the modification comprises a substitution at a position corresponding to I16, L35, M45, P73, D76, D79, A192, I100, A148, A163+G172, L268, V281, D285, L321, F297, N305, K316, S573, A341, M378, A381, F389, A483, A486, I510, A564, F586, K589, F636, K645, A629, and/or T681 such as to improve hydrogen bond contact, preferably a substitution corresponding to
- 20 I16T/D/N, L35Q, M45K, P73Q, D76E, D79E/Y, A192S/D/N, I100T/S/D/N/E/Q, A148D/N/E/Q/S/T/R/K, A163Y+G172S/D/N, L268R/K, V281/Q, D285R/K, L321Q, F297N/D/Q/E, N305K/R, K316N/D, S573N/D, A341R/K, M378R/K, A381S/D/N, F389Y, A483S/D/N, A486Q/E, I510R/K, A564S/D/N, F586S/D/N, K589S/D/Q/N, F636Y, K645T, A629N/D/E/Q, and/or T681D/N/E/Q/S.
- 25 16. The polypeptide of any of claims 11-15, wherein the modification comprises substitutions such as to introduce one or more interdomain disulfide bonds, preferably corresponding to G236C + S583C, G618C + R272C, and/or A348C + V487C.
17. The polypeptide of any of claims 11-16, wherein the substitution at a position corresponding to L51, L75, L78, G88, G91, T94, V114, I125, V126, T134, G157,
- 30 L217, S235, G236, V254, V279, V281, L286, V289, I290, V308, L321, I325, D326, L343, F349, S353, I359, I405, L448, Q449, L452, I470, G509, V515, S583, G625, L627, L628 and/or A670 so as to fill an internal cavity or crevice, preferably a substitution corresponding to L51W, L75F/Y, L78I, G88A/V/T, G91T/S/V/N, T94V/I/L, V114V/I/L, I125L/M/F/Y/W, V126I/L, T134V/I/L/M/F/Y/W, G157A/V/I/L,
- 35 L217V/I/M/F/Y/W, S235I/L/M/F/Y/W, G236A/V/I/L/M/F/Y/W, V254I/L/M/F/Y/W,

V279M/I/L/F, V281I/L/M/F/Y/W, L286F, V289I/L/R, I290M/L/F, V308I/L/M/F/Y/W, L321I/M/F/Y/W, I325L/M/F/Y/W, D326E/Q, L343M/F/Y/W, F349W/Y, S353V/I/L, I359L/M/F/Y/W, I405M/L/Y/F/W, L448Y, Q449Y, L452M/Y/F/W, I470M/L/F, G509A/V/I/L/M/S/T/D/N, V515I/L, S583V/I/L/V, G625A/V/I/L/M/F/Y/W, L627M/F/Y, 5 L628M/I/F/Y/W, A670V/I/L/M/F/Y/W and/or L217 in combination with L75 (e.g. L217F/Y in combination with L75F/Y).

18. The polypeptide of any of claims 11-17, wherein the modification comprises a substitution at a position corresponding to N106, N320 and Q624 so as to create a salt bridge, preferably a substitution corresponding to N106R, N320E/D and/or 10 Q624E.

19. The polypeptide of any of claims 11-18, wherein the modification comprises a substitution at a position corresponding to K244 and/or K316 such as to alter the charge distribution, preferably a substitution corresponding to K244S and/or K316G/N/D.

15 20. The polypeptide of any of claims 11-19, wherein the modification comprises a substitution at a position corresponding to V281 and/or A629 such as to alter the binding site, preferably a substitution corresponding to V281Q and/or A629N/D/E/Q.

21. The polypeptide of any of claims 11-20, wherein the modification comprises substitutions such as to alter the interdomain interaction at a position corresponding 20 to F143+F194+L78, A341+A348+L398+I415+T439+L464+L465, L557, S240+L268, Q208+L628, F427+Q500+N507+M508+S573 and/or I510+V620, preferably substitutions corresponding to F143Y+F194Y+L78Y/F/W/E/Q, A341S/D/N+A348V/I/L+L398E/Q/N/D+I415E/Q+T439D/E/Q/N+L464D/E+L465D/E/N/Q/R/K, L557Q/E/N/D, S240D/E/N/Q+L268D/E/N/Q/R/K, Q208D/E/Q+L628E/Q/N/D, 25 F427E/Q/R/K/Y+Q500Y+N507Q/E/D+M508K/R/E/Q+S573D/E/N/Q; and/or I510D/E/N/Q/S+V620D/E/N/Q.

22. A polypeptide which:

- a) has maltogenic alpha-amylase activity;
- b) has at least 70 % identity to SEQ ID NO: 1;
- 30 c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to P191, A192, G193, F194 and/or S195; and
- d) has higher specific amylase activity than the polypeptide of SEQ ID NO: 1.

23. The polypeptide of claim 22, wherein the modification comprises a deletion, preferably the deletion Δ (191-195).

24. The polypeptide of claim 22, wherein the modification comprises insertion, preferably 192-A-193.

5 25. A polypeptide which:

- a) has maltogenic alpha-amylase activity;
- b) has at least 70 % identity to SEQ ID NO: 1;
- c) comprises an amino acid modification compared to SEQ ID NO: 1 at a position corresponding to A30, K40, N115, T142, F188, T189, P191, A192, 10 G193, F194, S195, D261, T288, N327, K425, K520 and/or N595; and
- d) has a higher ability than the polypeptide of SEQ ID NO: 1 to reduce retrogradation of starch and/or staling of bread.

26. The polypeptide of claim 26, wherein the modification comprises A30D, K40R, N115D, T142A F188L, T189Y, Δ (191-195), D261G, T288P, N327S, K425E, K520R 15 and/or N595I.

27. A nucleic acid sequence encoding the polypeptide of any of claims 9-26, preferably operably linked to one or more control sequences which direct the expression of the variant in a suitable expression host.

28. A recombinant expression vector comprising the nucleic acid sequence of 20 claim 27, a promoter, and transcriptional and translational stop signals, and preferably further comprising a selectable marker.

29. A transformed host cell comprising the nucleic acid sequence of claim 27 or the vector of claim 28.

30. A method for producing the polypeptide of any of claims 9-26, comprising: 25 a) cultivating the transformed host cell of claim 29 under conditions conducive to expression of the variant; and b) recovering the variant.

31. A process for preparing a dough or a baked product prepared from the dough which comprises adding the polypeptide of any of claims 9-26, or a variant produced

by the method of any of claims 1-8 to the dough in an amount which is effective to retard the staling of the bread.

32. The process of claim 31, wherein the variant is added in an amount of 0.1-5 mg per kg of flour, preferably 0.5-2 mg/kg.

1/1

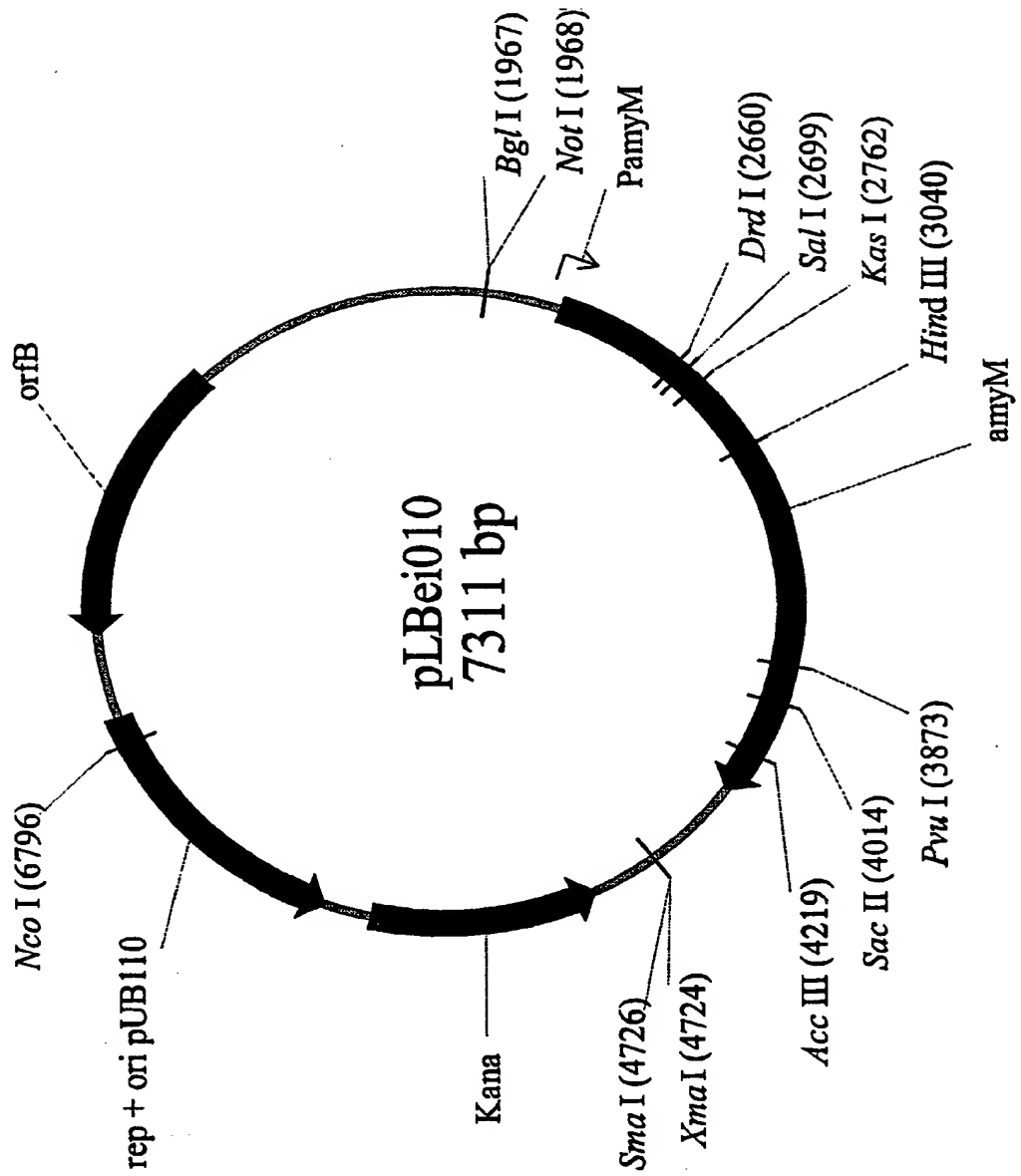


Fig. 1

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| | | | | | | | | | | | | | | | | |
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| | | | | | | | | | | | | | | | | |
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Asp Phe Lys Gln Ile Glu Glu His Phe Gly Asn Trp Thr Thr Phe Asp
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 Thr Leu Val Asn Asp Ala His Gln Asn Gly Ile Lys Val Ile Val Asp
 145 150 155 160
 Phe Val Pro Asn His Ser Thr Pro Phe Lys Ala Asn Asp Ser Thr Phe
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 Ala Glu Gly Gly Ala Leu Tyr Asn Asn Gly Thr Tyr Met Gly Asn Tyr
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 Phe Asp Asp Ala Thr Lys Gly Tyr Phe His His Asn Gly Asp Ile Ser
 195 200 205
 Asn Trp Asp Asp Arg Tyr Glu Ala Gln Trp Lys Asn Phe Thr Asp Pro
 210 215 220
 Ala Gly Phe Ser Leu Ala Asp Leu Ser Gln Glu Asn Gly Thr Ile Ala
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 Gln Tyr Leu Thr Asp Ala Ala Val Gln Leu Val Ala His Gly Ala Asp
 245 250 255
 Gly Leu Arg Ile Asp Ala Val Lys His Phe Asn Ser Gly Phe Ser Lys
 260 265 270
 Ser Leu Ala Asp Lys Leu Tyr Gln Lys Lys Asp Ile Phe Leu Val Gly
 275 280 285
 Glu Trp Tyr Gly Asp Asp Pro Gly Thr Ala Asn His Leu Glu Lys Val
 290 295 300
 Arg Tyr Ala Asn Asn Ser Gly Val Asn Val Leu Asp Phe Asp Leu Asn
 305 310 315 320
 Thr Val Ile Arg Asn Val Phe Gly Thr Phe Thr Gln Thr Met Tyr Asp
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 Asn Leu Ile Thr Phe Ile Asp Asn His Asp Met Ser Arg Phe Leu Ser
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 Val Asn Ser Asn Lys Ala Asn Leu His Gln Ala Leu Ala Phe Ile Leu
 370 375 380

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| Thr Ser Arg Gly Thr Pro Ser Ile Tyr Tyr Gly Thr Glu Gln Tyr Met | | | |
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| Ala Gly Gly Asn Asp Pro Tyr Asn Arg Gly Met Met Pro Ala Phe Asp | | | |
| | 405 | 410 | 415 |
| Thr Thr Thr Thr Ala Phe Lys Glu Val Ser Thr Leu Ala Gly Leu Arg | | | |
| | 420 | 425 | 430 |
| Arg Asn Asn Ala Ala Ile Gln Tyr Gly Thr Thr Thr Gln Arg Trp Ile | | | |
| | 435 | 440 | 445 |
| Asn Asn Asp Val Tyr Ile Tyr Glu Arg Lys Phe Phe Asn Asp Val Val | | | |
| | 450 | 455 | 460 |
| Leu Val Ala Ile Asn Arg Asn Thr Gln Ser Ser Tyr Ser Ile Ser Gly | | | |
| | 465 | 470 | 475 |
| Leu Gln Thr Ala Leu Pro Asn Gly Ser Tyr Ala Asp Tyr Leu Ser Gly | | | |
| | 485 | 490 | 495 |
| Leu Leu Gly Gly Asn Gly Ile Ser Val Ser Asn Gly Ser Val Ala Ser | | | |
| | 500 | 505 | 510 |
| Phe Thr Leu Ala Pro Gly Ala Val Ser Val Trp Gln Tyr Ser Thr Ser | | | |
| | 515 | 520 | 525 |
| Ala Ser Ala Pro Gln Ile Gly Ser Val Ala Pro Asn Met Gly Ile Pro | | | |
| | 530 | 535 | 540 |
| Gly Asn Val Val Thr Ile Asp Gly Lys Gly Phe Gly Thr Thr Gln Gly | | | |
| | 545 | 550 | 555 |
| Thr Val Thr Phe Gly Gly Val Thr Ala Thr Val Lys Ser Trp Thr Ser | | | |
| | 565 | 570 | 575 |
| Asn Arg Ile Glu Val Tyr Val Pro Asn Met Ala Ala Gly Leu Thr Asp | | | |
| | 580 | 585 | 590 |
| Val Lys Val Thr Ala Gly Gly Val Ser Ser Asn Leu Tyr Ser Tyr Asn | | | |
| | 595 | 600 | 605 |
| Ile Leu Ser Gly Thr Gln Thr Ser Val Val Phe Thr Val Lys Ser Ala | | | |
| | 610 | 615 | 620 |
| Pro Pro Thr Asn Leu Gly Asp Lys Ile Tyr Leu Thr Gly Asn Ile Pro | | | |
| | 625 | 630 | 635 |
| | | | 640 |

Glu Leu Gly Asn Trp Ser Thr Asp Thr Ser Gly Ala Val Asn Asn Ala
 645 650 655

Gln Gly Pro Leu Leu Ala Pro Asn Tyr Pro Asp Trp Phe Tyr Val Phe
 660 665 670

Ser Val Pro Ala Gly Lys Thr Ile Gln Phe Lys Phe Phe Ile Lys Arg
 675 680 685

Ala Asp Gly Thr Ile Gln Trp Glu Asn Gly Ser Asn His Val Ala Thr
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Thr Pro Thr Gly Ala Thr Gly Asn Ile Thr Val Thr Trp Gln Asn
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<223> Description of Artificial Sequence: B 346 Primer

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22

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 99/00088

| A. CLASSIFICATION OF SUBJECT MATTER | | |
|---|--|--|
| IPC6: C12N 9/28, A21D 8/04 According to International Patent Classification (IPC) or to both national classification and IPC | | |
| B. FIELDS SEARCHED | | |
| Minimum documentation searched (classification system followed by classification symbols) | | |
| IPC6: C12N | | |
| Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched | | |
| SE,DK,FI,NO classes as above | | |
| Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) | | |
| C. DOCUMENTS CONSIDERED TO BE RELEVANT | | |
| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
| X | WO 9623874 A1 (NOVO NORDISK A/S), 8 August 1996 (08.08.96), see page 30-37, claims 1-2 -- | 1-32 |
| X | WO 9743424 A1 (GENENCOR INTERNATIONAL, INC.), 20 November 1997 (20.11.97), see page 3, lines 21-34, page 12, lines 15-19 -- | 1-8 |
| A | -- | 7-32 |
| X | WO 9741213 A1 (NOVO NORDISK A/S), 6 November 1997 (06.11.97), see page 11, lines 5-12 -- | 1-8 |
| A | -- | 9-32 |
| <input checked="" type="checkbox"/> Further documents are listed in the continuation of Box C. <input checked="" type="checkbox"/> See patent family annex. | | |
| * Special categories of cited documents: "A" document defining the general state of the art which is not considered to be of particular relevance "E" earlier document but published on or after the international filing date "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) "O" document referring to an oral disclosure, use, exhibition or other means "P" document published prior to the international filing date but later than the priority date claimed "T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention "X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone "Y" document of particular relevance: the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art "&" document member of the same patent family | | |
| Date of the actual completion of the international search | | Date of mailing of the international search report |
| 8 June 1999 | | 08 -06- 1999 |
| Name and mailing address of the ISA/ Swedish Patent Office Box 5055, S-102 42 STOCKHOLM Facsimile No. +46 8 666 02 86 | | Authorized officer Yvonne Siösteen Telephone No. +46 8 782 25 00 |

INTERNATIONAL SEARCH REPORT

International application No.

PCT/DK 99/00088

| C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT | | |
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| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
| A | Databas Swissprot, accessionno. P19531, Diderichsen B. et al: "Maltogenicalpha- amylase precursor (EC 3.2.1.133) Glucan 1,4-alpha-maltohydrolase"; & Fems Microbiol. Lett. 56:53-60 (1988) -- | 1-32 |
| A | Dialog Information Services, file 5, Biosis Previews, Dialog accession no. 07281496, Biosis accession no. 000090061383, Boel E et al: "Calcium binding in alpha amylases an X-ray diffraction study at 2.1-Aresolution of two enzymes from aspergillus"; & Biochemistry 29 (26). 1990. 6244-6249 -- | 1-32 |
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| A | J. Mol. Biol., Volume 229, 1993, Changsoo Chang et al, "Crystallization and Preliminary X-ray Crystallographic Analysis of alpha-Amylase from Bacillus subtilis" page 235 - page 238 -- | 1-32 |
| A | Plant Molecular Biology, Volume 25, 1994, Birte Svensson, "Protein engineering in the alpha-amylase family: catalytic mechanism, substrate specificity, and stability" page 141 - page 157 -- ----- | 1-32 |

INTERNATIONAL SEARCH REPORT

Information on patent family members

03/05/99

International application No.

PCT/DK 99/00088

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
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| WO 9623874 A1 | 08/08/96 | AU 4483496 A BR 9607013 A CA 2211316 A CN 1172501 A EP 0808363 A JP 11500003 T | 21/08/96 28/10/97 08/08/96 04/02/98 26/11/97 06/01/99 |
| WO 9743424 A1 | 20/11/97 | AU 2996997 A US 5763385 A | 05/12/97 09/06/98 |
| WO 9741213 A1 | 06/11/97 | AU 2692897 A EP 0904360 A | 19/11/97 31/03/99 |